Latest

10690708.trn

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LOGINID: SSSPTA1626GMS

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TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
      2
                 "Ask CAS" for self-help around the clock
                 The Derwent World Patents Index suite of databases on STN
NEWS
         OCT 23
                 has been enhanced and reloaded
                 CHEMLIST enhanced with new search and display field
NEWS
         OCT 30
NEWS
         NOV 03
                 JAPIO enhanced with IPC 8 features and functionality
NEWS
         NOV 10
                 CA/CAplus F-Term thesaurus enhanced
NEWS
         NOV 10
                 STN Express with Discover! free maintenance release Version
                 8.01c now available
NEWS
         NOV 20
                 CA/CAplus to MARPAT accession number crossover limit increased
                 to 50,000
NEWS
         DEC 01
                 CAS REGISTRY updated with new ambiguity codes
                 CAS REGISTRY chemical nomenclature enhanced
NEWS 10
         DEC 11
                 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 11
         DEC 14
                 GBFULL and FRFULL enhanced with IPC 8 features and
NEWS 12
        DEC 14
                 functionality
NEWS 13
         DEC 18
                 CA/CAplus pre-1967 chemical substance index entries enhanced
                 with preparation role
         DEC 18
NEWS 14
                 CA/CAplus patent kind codes updated
NEWS 15
        DEC 18
                 MARPAT to CA/CAplus accession number crossover limit increased
                 to 50,000
NEWS 16
        DEC 18
                 MEDLINE updated in preparation for 2007 reload
NEWS 17
        DEC 27
                 CA/CAplus enhanced with more pre-1907 records
        JAN 08
NEWS 18
                 CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 19
        JAN 16
                 CA/CAplus Company Name Thesaurus enhanced and reloaded
        JAN 16
NEWS 20
                 IPC version 2007.01 thesaurus available on STN
        JAN 16
NEWS 21
                 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
         JAN 22
                 CA/CAplus updated with revised CAS roles
NEWS 22
         JAN 22
NEWS 23
                 CA/CAplus enhanced with patent applications from India
NEWS 24
        JAN 29
                 PHAR reloaded with new search and display fields
NEWS 25
        JAN 29
                 CAS Registry Number crossover limit increased to 300,000 in
                 multiple databases
NEWS 26
        FEB 13
                 CASREACT coverage to be extended
NEWS 27
        Feb 15
                 PATDPASPC enhanced with Drug Approval numbers
NEWS 28 Feb 15
                 RUSSIAPAT enhanced with pre-1994 records
NEWS 29
        Feb 23
                 KOREAPAT enhanced with IPC 8 features and functionality
NEWS 30 Feb 26
                MEDLINE reloaded with enhancements
NEWS 31 Feb 26
                EMBASE enhanced with Clinical Trial Number field
NEWS 32
        Feb 26
                 TOXCENTER enhanced with reloaded MEDLINE
NEWS 33
        Feb 26
                 IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 34
        Feb 26
                 CAS Registry Number crossover limit increased from 10,000
                 to 300,000 in multiple databases
```

NEWS EXPRESS NOVEMBER 10 -CURRENT WINDOWS VERSION IS V8.01c, CURRENT

MACINTOSH VERSION IS V6.0c(ENG) AND V6.0jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

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NEWS IPC8 For general information regarding STN implementation of IPC 8

NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.84 0.84

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 12:45:37 ON 13 MAR 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 12 MAR 2007 HIGHEST RN 926069-79-6 DICTIONARY FILE UPDATES: 12 MAR 2007 HIGHEST RN 926069-79-6

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10690708.str

chain nodes : 16 17 18 19 20 21 22 23 24 ring nodes : 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 chain bonds : 3-16 5-23 13-18 14-24 15-17 16-17 16-21 17-19 17-20 21-22 ring bonds : 1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 3-16 5-9 8-9 15-17 16-17 16-21 17-19 17-20 exact bonds : 5-6 5-23 6-7 13-18 14-24 21-22 normalized bonds : 1-2 1-7 2-3 3-4 4-8 7-8 10-11 10-15 11-12 12-13 13-14 14-15 isolated ring systems : containing 1 : 10 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1

L2

L3

SAMPLE SEARCH INITIATED 12:45:53 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -1 TO ITERATE

100.0% PROCESSED

1 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

1 TO 80 0 TO

PROJECTED ANSWERS:

0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 12:46:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -

50 TO ITERATE

100.0% PROCESSED

50 ITERATIONS

SEARCH TIME: 00.00.01

1 SEA SSS FUL L1

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY 172.10

SESSION 172.94

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 12:46:06 ON 13 MAR 2007

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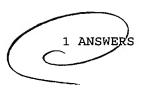
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FILE COVERS 1907 - 13 Mar 2007 VOL 146 ISS 12 FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

AUTHOR (S):

L4 3 L3

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:476237 HCAPLUS

DOCUMENT NUMBER: 145:137256

TITLE: The Discovery of New 11β-Hydroxysteroid

Dehydrogenase Type 1 Inhibitors by Common Feature

Pharmacophore Modeling and Virtual Screening Schuster, Daniela; Maurer, Evelyne M.; Laggner,

Christian; Nashev, Lyubomir G.; Wilckens, Thomas;

Langer, Thierry; Odermatt, Alex

CORPORATE SOURCE: Institute of Pharmacy, Department of Pharmaceutical

Chemistry, University of Innsbruck, Innsbruck, 6020,

Austria

SOURCE: Journal of Medicinal Chemistry (2006), 49(12),

3454-3466

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: Southai

GI

AB 11β -Hydroxysteroid dehydrogenase (11 β -HSD) enzymes catalyze the conversion of biol. inactive 11-ketosteroids into their active

Ι

 11β -hydroxy derivs. and vice versa. Inhibition of 11β -HSD1 has considerable therapeutic potential for glucocorticoid-associated diseases including obesity, diabetes, wound healing, and muscle atrophy. Because inhibition of related enzymes such as 11 β -HSD2 and 17 β -HSDs causes sodium retention and hypertension or interferes with sex steroid. hormone metabolism, resp., highly selective 11β-HSD1 inhibitors are required for successful therapy. Here, the authors employed the software package Catalyst to develop ligand-based multifeature pharmacophore models for 11β -HSD1 inhibitors. Virtual screening expts. and subsequent in vitro evaluation of promising hits revealed several selective inhibitors. Efficient inhibition of recombinant human 11β-HSD1 in intact transfected cells as well as endogenous enzyme in mouse 3T3-L1 adipocytes and C2C12 myotubes was demonstrated for compound (I), which was able to block subsequent cortisol-dependent activation of glucocorticoid receptors with only minor direct effects on the receptor itself. Our results suggest that inhibitor-based pharmacophore models for 118-HSD1 in combination with suitable cell-based activity assays, including such for related enzymes, can be used for the identification of selective and potent inhibitors.

IT 686746-36-1

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(discovery of new hydroxysteroid dehydrogenase inhibitors by common feature pharmacophore modeling and virtual screening)

RN 686746-36-1 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-ethyl-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:261388 HCAPLUS

DOCUMENT NUMBER: 144:460298

TITLE: Benzothiazole derivatives as novel inhibitors of human

118 hydroxysteroid dehydrogenase type 1

AUTHOR(S): Su, Xiangdong; Vicker, Nigel; Ganeshapillai,

Bharshini; Smith, Andrew; Purohit, Atul; Reed, Michael

J.; Potter, Barry V. L.

CORPORATE SOURCE: Medicinal Chemistry, Department of Pharmacy and

Pharmacology and Sterix Ltd., University of Bath,

Bath, BA2 7AY, UK

SOURCE: Molecular and Cellular Endocringlogy (2006), 248(1-2)

214-217

CODEN: MCEND6; ISSN: 0303-7207

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

AB Selective inhibitors of 11β -hydroxysteroid dehydrogenase type 1 (11 β -HSD1) have considerable potential as treatments for metabolic diseases, such as diabetes mellitus type 2 or obesity. Here, we report

the discovery and synthesis of a series of novel benzothiazole derivs. and their inhibitory activities against 11 β -HSD1 from human hepatic microsomes measured using a RIA method. The benzothiazole derivs. 1 and 2 showed greater than 80% inhibition for 11 β -HSD1 at 10 μM and exhibited IC50 values in the low micromolar range. The preliminary SAR study suggested the introduction of a chlorine substituent at the 4 position of the benzothiazole ring greatly enhanced the inhibitory activities. Docking studies with the benzothiazole derivative 1 into the crystal structure of human 11 β -HSD1 revealed how the mol. may interact with the enzyme and cofactor.

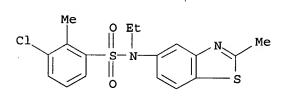
IT 686746-36-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(benzothiazole derivs. as inhibitors of human 11β -hydroxysteroid dehydrogenase type 1)

RN 686746-36-1 HCAPLUS

Benzenesulfonamide, 3-chloro-N-ethyl-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

11

ACCESSION NUMBER:

DOCUMENT NUMBER:

140:391280

TITLE:

CN

Preparation of arylsulfonylbenzazoles as inhibitors of

11-β-hydroxy steroid dehydrogenase type 1 and

type 2.

INVENTOR (S):

Vicker, Nigel; Sw., Xiangdong; Ganeshapillai,

Dharshini; Purchit, Atul; Reed, Michael John; Potter,

Barry Victor Lloyd Sterix Limited, UK

2004:368925 HCAPLUS

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 172 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT N | ю. | | | KIN | D : | DATE | | | APPL | ICAT | ION I | NO. | | D | ATE | |
|----------|-----|-----|-------------|-----------|-----|----------------|-----|-----|------|------|----------|-----|-----|-----|-----|-----|
| | | | | <i></i>) | |) | | | | | | | | | | |
| | | | A1 20040506 | | | WO 2003-GB4590 | | | | | 20031023 | | | | | |
| W: | ΑE, | AG, | AL, | AM, | AT, | `AU, | ΔŽ, | BA, | BB, | BG, | BR, | BY, | BZ, | CA, | CH, | CN, |
| | CO, | CR, | CU, | CZ, | DÉ | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, | GE, |
| | GH, | GM, | HR, | ΗU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KP, | KR, | KZ, | LC, | LK, |
| | LR, | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NI, | NO, | NZ, |
| | OM, | PG, | PH, | ΡL, | PT, | RO, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SY, | ТJ, | TM, |
| | | | | | | | | | VC, | | | | | | - | |
| | | | | | | | | | SZ, | | | | | | | |
| | KG, | KZ, | MD, | RU, | TJ, | TM, | ΑT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, |
| | FI, | FR, | GB, | GR, | HU, | ΙE, | IT, | LU, | MC, | NL, | PT, | RO, | SE, | SI, | SK, | TR, |

| BF | BJ, CF | CG, | CI, CM, | GA, | GN, G | Q, GW, | ML, | MR, | NE, | SN, | TD, | TG |
|------------------|------------|--------|---------------------------------------|-------|--------|--------|-------|------|-----|-----|------|-----|
| CA 2501228 | | A1 | | 0506 | | 2003- | | | | | 0031 | |
| AU 2003274 | 373 | A1 | 2004 | 0513 | AU | 2003- | 2743 | 73 | | 2 | 0031 | 023 |
| US 2004143 | | A1 | | 0722 | US | 2003- | 6907 | 08 | | 2 | 0031 | 023 |
| EP 1556040 | ı | A1 | 2005 | 0727 | EP | 2003- | 7583 | 57 | | 2 | 0031 | 023 |
| R: AT | ', BE, CH, | DE, | DK, ES, | FR, | GB, GF | R, IT, | LI, | LU, | NL, | SE, | MC, | PT, |
| IB | , SI, LT, | LV, | FI, RO, | MK, | CY, AI | J, TR, | BG, | CZ, | EE, | HU, | SK | |
| BR 2003015 | 605 | Α | 2005 | 0830 | BR | 2003- | 1560 | 5 | | 2 | 0031 | 023 |
| CN 1723022 | | Α | 2006 | 0118 | CN | 2003- | 8010 | 5509 | | 2 | 0031 | 023 |
| JP 2006514 | | | | 0511 | JP | 2004- | 5461 | 83 | | 2 | 0031 | 023 |
| NO 2005002 | | Α | 2005 | 0722 | NO | 2005- | 2469 | | | 2 | 0050 | 523 |
| PRIORITY APPLN. | INFO.: | | | | GB | 2002- | 2483 | 0 | 1 | A 2 | 0021 | 024 |
| | | | | | US | 2002- | 43663 | 35P | 0 | P 2 | 0021 | 230 |
| | | | | | WO | 2003- | GB45 | 90 | 1 | W 2 | 0031 | 023 |
| OBUDE COIDER (C) | | 343 73 | D D D D D D D D D D D D D D D D D D D | 20101 | 2.0 | | | | | | | |

OTHER SOURCE(S):

MARPAT 140:391280

GI

AB Title compds. [I; 1 of R1, R2 = R5SO2N(R4)L; R4 = H, hydrocarbyl; R5 = hydrocarbyl; L = optional linker group; R1R2 = atoms form a ring; X = S, O, NR6, C(R7)(R8); R6-R8 = H, hydrocarbyl], were prepared Thus, title compound (II) inhibited 11β -HSD1 with IC50 = 6.6 μM.

IT 686746-36-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indoles, benzothiazoles, benzoxazoles, and benzimidazoles as inhibitors of hydroxy steroid dehydrogenase)

RN 686746-36-1 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-ethyl-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

=> FIL REGISTRY COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 31.41 204.35

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

INTRY SESSION
-2.34 -2.34

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http://www.cas.org/ONLINE/UG/regprops.html

=>

Uploading C:\Program Files\Stnexp\Queries\10690708a.str

chain nodes :

16 17 18 19 21

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds :

3-16 15-17 16-17 16-21 17-18 17-19

ring bonds :

1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

3-16 5-9 8-9 15-17 16-17 17-18 17-19

exact bonds :

5-6 6-7 16-21

normalized bonds :

1-2 1-7 2-3 3-4 4-8 7-8 10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems :

containing 1 : 10 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

· STR L5

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 12:50:17 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 33 TO 447

PROJECTED ANSWERS: 0 TO 0

0 SEA SSS SAM L5

=> s 15 sss full

FULL SEARCH INITIATED 12:50:25 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 296 TO ITERATE

100.0% PROCESSED 296 ITERATIONS 52 ANSWERS

03/13/2007 Page 10

SEARCH TIME: 00.00.02

L7 52 SEA SSS FUL L5

=> FIL HCAPLUS

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
172.10
376.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -2.34

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FILE COVERS 1907 - 13 Mar 2007 VOL 146 ISS 12 FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17

L8 8 L7

=> FIL REGISTRY

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
15.60 392.05

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION

CA SUBSCRIBER PRICE

0.00
-2.34

FILE 'REGISTRY' ENTERED AT 12:54:09 ON 13 MAR 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 12 MAR 2007 HIGHEST RN 926069-79-6 DICTIONARY FILE UPDATES: 12 MAR 2007 HIGHEST RN 926069-79-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

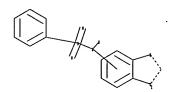
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>

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chain nodes :

16 17 18 19 21

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds :

15-17 16-21 16-17 17-18 17-19

ring bonds :

1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

exact/norm bonds :

5-6 5-9 6-7 8-9 15-17 16-21 16-17 17-18 17-19

normalized bonds :

1-2 1-7 2-3 3-4 4-8 7-8 10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems :

containing 1 : 10 :

G1:0,S,N,CH2,NH

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS 23:Atom

L9 STRUCTURE UPLOADED

=> d 19

L9 HAS NO ANSWERS

L9 STR

G1 O, S, N, CH2, NH

Structure attributes must be viewed using STN Express query preparation.

32 ANSWERS

=> s 19

SAMPLE SEARCH INITIATED 12:54:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5559 TO ITERATE

36.0% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 106710 TO 115650

PROJECTED ANSWERS: 1213 TO 2343

L10 32 SEA SSS SAM L9

=> s 19 sss full

FULL SEARCH INITIATED 12:54:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 114915 TO ITERATE

100.0% PROCESSED 114915 ITERATIONS 1585 ANSWERS

SEARCH TIME: 00.00.01

L11 1585 SEA SSS FUL L9

=> FIL HCAPLUS

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 172.10 564.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY TOTAL SESSION

CA SUBSCRIBER PRICE

0.00

-2.34

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FILE COVERS 1907 - 13 Mar 2007 VOL 146 ISS 12 FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L1

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(FILE 'HOME' ENTERED AT 12:43:35 ON 13 MAR 2007)

FILE 'REGISTRY' ENTERED AT 12:45:37 ON 13 MAR 2007

STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:46:06 ON 13 MAR 2007

L4 3 S L3

FILE 'REGISTRY' ENTERED AT 12:49:59 ON 13 MAR 2007

STRUCTURE UPLOADED

L6 0 S L5

L7 52 S L5 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:50:33 ON 13 MAR 2007

L8 8 S L7

FILE 'REGISTRY' ENTERED AT 12:54:09 ON 13 MAR 2007

STRUCTURE UPLOADED

L10 32 S L9

L11 1585 S L9 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:54:48 ON 13 MAR 2007

=> s 111

L12 184 L11

=> s 112 and py<=2002 22869925 PY<=2002

L13 134 L12 AND PY<=2002

=> s l13 and us/pc 1643942 US/PC

L14 39 L13 AND US/PC

=> s l14 and p/dt 5633762 P/DT

L15 39 L14 AND P/DT

=> d 18 ibib abs hitstr tot

L8 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:476237 HCAPLUS

DOCUMENT NUMBER: 145:137256

TITLE: The Discovery of New 11 β -Hydroxysteroid

Dehydrogenase Type 1 Inhibitors by Common Feature

Pharmacophore Modeling and Virtual Screening Schuster, Daniela; Maurer, Evelyne M.; Laggner, Christian; Nashev, Lyubomir G.; Wilckens, Thomas;

Langer, Thierry; Odermatt, Alex

CORPORATE SOURCE: Institute of Pharmacy, Department of Pharmaceutical

Chemistry, University of Innsbruck, Innsbruck, 6020,

Austria

SOURCE: Journal of Medicinal Chemistry (2006), 49 (12),

3454-3466

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

AUTHOR (S):

AB 11 β -Hydroxysteroid dehydrogenase (11 β -HSD) enzymes catalyze the conversion of biol. inactive 11-ketosteroids into their active 11 β -hydroxy derivs. and vice versa. Inhibition of 11 β -HSD1 has considerable therapeutic potential for glucocorticoid-associated diseases including obesity, diabetes, wound healing, and muscle atrophy. Because inhibition of related enzymes such as 11 β -HSD2 and 17 β -HSDs causes sodium retention and hypertension or interferes with sex steroid hormone metabolism, resp., highly selective 11 β -HSD1 inhibitors are required for successful therapy. Here, the authors employed the software package Catalyst to develop ligand-based multifeature pharmacophore models for 11 β -HSD1 inhibitors. Virtual screening expts. and subsequent in vitro evaluation of promising hits revealed several selective inhibitors.

Т

Efficient inhibition of recombinant human 11 β -HSD1 in intact transfected cells as well as endogenous enzyme in mouse 3T3-L1 adipocytes and C2C12 myotubes was demonstrated for compound (I), which was able to block subsequent cortisol-dependent activation of glucocorticoid receptors with only minor direct effects on the receptor itself. Our results suggest that inhibitor-based pharmacophore models for 11 β -HSD1 in combination with suitable cell-based activity assays, including such for related enzymes, can be used for the identification of selective and potent inhibitors.

IT 670272-62-5 671200-96-7 686746-30-5 686746-31-6 686746-32-7 686746-33-8 686746-34-9 686746-37-2 686746-38-3 686746-39-4 686746-40-7 686746-41-8 686746-44-1 686746-45-2 686746-47-4 686746-45-5 686746-51-0 686746-52-1 686746-53-2 686746-54-3 686746-55-4 686746-56-5 686746-57-6 686746-58-7 686746-82-7 686746-87-2

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(discovery of new hydroxysteroid dehydrogenase inhibitors by common feature pharmacophore modeling and virtual screening)

RN 670272-62-5 HCAPLUS

RN 671200-96-7 HCAPLUS

CN Benzenesulfonamide, 2,3,5,6-tetramethyl-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-30-5 HCAPLUS

CN Benzenesulfonamide, 2,4-dichloro-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-31-6 HCAPLUS

CN Benzenesulfonamide, 3-chloro-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-32-7 HCAPLUS

CN Benzenesulfonamide, N-(2-methyl-5-benzothiazolyl)-4-propyl- (9CI) (CA INDEX NAME)

RN 686746-33-8 HCAPLUS

CN Benzenesulfonamide, 4-methoxy-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-34-9 HCAPLUS

CN Benzenesulfonamide, 2-chloro-6-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-37-2 HCAPLUS

RN 686746-38-3 HCAPLUS

CN [1,1'-Biphenyl]-4-sulfonamide, N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-39-4 HCAPLUS

CN Benzenesulfonamide, 2,4,6-trichloro-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-40-7 HCAPLUS

CN Benzenesulfonamide, 4-bromo-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-41-8 HCAPLUS

CN Benzamide, 3,5-dichloro-N-(2-methyl-5-benzothiazolyl)-2-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]- (9CI) (CA INDEX NAME)

RN 686746-44-1 HCAPLUS

CN Benzoic acid, 3,5-dichloro-2-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]-(9CI) (CA INDEX NAME)

RN 686746-45-2 HCAPLUS

CN Benzenesulfonamide, 2,5-dichloro-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-47-4 HCAPLUS

CN Benzenesulfonamide, 5-chloro-2-methoxy-N-(2-methyl-5-benzothiazolyl)(9CI) (CA INDEX NAME)

RN 686746-48-5 HCAPLUS

CN Benzenesulfonamide, 2-cyano-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA

INDEX NAME)

RN 686746-49-6 HCAPLUS

CN Benzenesulfonamide, 2-methoxy-4-methyl-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-50-9 HCAPLUS

CN Benzenesulfonamide, 2-acetyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-51-0 HCAPLUS

.CN Benzenesulfonamide, N-(2-methyl-5-benzothiazolyl)-2,4,6-tris(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 686746-52-1 HCAPLUS

CN Benzenesulfonamide, N-(2-methyl-5-benzothiazolyl)-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 686746-53-2 HCAPLUS

CN Benzoic acid, 2-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 686746-54-3 HCAPLUS

CN Benzenesulfonamide, 3,4-dimethoxy-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-55-4 HCAPLUS

CN Benzenesulfonamide, 4-methoxy-2,3,5,6-tetramethyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-56-5 HCAPLUS

CN Benzenesulfonamide, 4-(1,1-dimethylethyl)-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-57-6 HCAPLUS

CN Benzenesulfonamide, 2,3,4,5,6-pentamethyl-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-58-7 HCAPLUS

CN Acetamide, N-[4-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 686746-59-8 HCAPLUS

CN Benzenesulfonamide, 2,3,4,5,6-pentafluoro-N-(2-methyl-5-benzothiazolyl)(9CI) (CA INDEX NAME)

RN 686746-70-3 HCAPLUS

CN Benzenesulfonamide, 2,5-dichloro-N-(4-chloro-2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

10690708.trn ·

RN 686746-71-4 HCAPLUS

CN Benzenesulfonamide, N-(4-chloro-2-methyl-5-benzothiazolyl)-4-propyl- (9CI) (CA INDEX NAME)

RN 686746-82-7 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-(4-chloro-2-methyl-5-benzothiazolyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 686746-87-2 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-(4,6-dichloro-2-methyl-5-benzothiazolyl)-2-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:261388 HCAPLUS

DOCUMENT NUMBER:

144:460298

TITLE:

Benzothiazole derivatives as novel inhibitors of human

11β-hydroxysteroid dehydrogenase type 1

AUTHOR (S):

Su, Xiangdong; Vicker, Nigel; Ganeshapillai,

Dharshini; Smith, Andrew; Purohit, Atul; Reed, Michael

J.; Potter, Barry V. L.

CORPORATE SOURCE: Medicinal Chemistry, Department of Pharmacy and

Pharmacology and Sterix Ltd., University of Bath,

Bath, BA2 7AY, UK

SOURCE: Molecular and Cellular Endocrinology (2006), 248(1-2)

214-217

CODEN: MCEND6; ISSN: 0303-7207

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

AB Selective inhibitors of 11β -hydroxysteroid dehydrogenase type 1 (11β -HSD1) have considerable potential as treatments for metabolic diseases, such as diabetes mellitus type 2 or obesity. Here, we report the discovery and synthesis of a series of novel benzothiazole derivs. and their inhibitory activities against 11β -HSD1 from human hepatic microsomes measured using a RIA method. The benzothiazole derivs. 1 and 2 showed greater than 80% inhibition for 11β -HSD1 at 10 μ M and exhibited IC50 values in the low micromolar range. The preliminary SAR study suggested the introduction of a chlorine substituent at the 4 position of the benzothiazole ring greatly enhanced the inhibitory activities. Docking studies with the benzothiazole derivative 1 into the crystal structure of human 11β -HSD1 revealed how the mol. may interact with the enzyme and cofactor.

IT 670272-62-5 686746-31-6 686746-32-7 686746-38-3 686746-40-7 686746-45-2

686746-70-3 686746-71-4 686746-82-7

886839-51-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(benzothiazole derivs. as inhibitors of human 11β -hydroxysteroid dehydrogenase type 1)

RN 670272-62-5 HCAPLUS

CN Benzenesulfonamide, N-(2-methyl-5-benzothiazolyl)-4-phenoxy- (9CI) (CA INDEX NAME)

RN 686746-31-6 HCAPLUS

CN Benzenesulfonamide, 3-chloro-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-32-7 HCAPLUS

CN Benzenesulfonamide, N-(2-methyl-5-benzothiazolyl)-4-propyl- (9CI) (CA INDEX NAME)

RN 686746-38-3 HCAPLUS

CN [1,1'-Biphenyl]-4-sulfonamide, N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-40-7 HCAPLUS

CN Benzenesulfonamide, 4-bromo-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-45-2 HCAPLUS

CN Benzenesulfonamide, 2,5-dichloro-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-70-3 HCAPLUS

CN Benzenesulfonamide, 2,5-dichloro-N-(4-chloro-2-methyl-5-benzothiazolyl)(9CI) (CA INDEX NAME)

RN 686746-71-4 HCAPLUS

CN Benzenesulfonamide, N-(4-chloro-2-methyl-5-benzothiazolyl)-4-propyl- (9CI) (CA INDEX NAME)

RN 686746-82-7 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-(4-chloro-2-methyl-5-benzothiazolyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 886839-51-6 HCAPLUS

CN Benzoic acid, 2,4-dichloro-5-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]-(9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2005:1042213 HCAPLUS

DOCUMENT NUMBER:

143:326199

TITLE:

Preparation of sulfonamides as inhibitors for collagen receptor integrins for treating thrombosis and cancer

INVENTOR(S):

Smith, David; Marjamaeki, Anne; Ojala, Marika; Pihlavisto, Marjo; Heino, Jyrki; Kaepylae, Jarmo;

Pentikaeinen, Olli; Nyroenen, Tommi; Johnson, Mark;

Huhtala, Mikko

PATENT ASSIGNEE(S): Biotie Therapies Corporation, Finland

SOURCE:

PCT Int. Appl., 61 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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PATENT NO.
                          KIND
                                  DATE
                                              APPLICATION NO.
                                                                       DATE
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                                 20050929
                                              WO 2004-FI160
     WO 2005090297
                           A1
                                                                       20040319
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
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             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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             TD, TG
     AU 2004317332
                                  20050929
                           A1
                                              AU 2004-317332
                                                                       20040712
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                                              CA 2004-2559919
                                                                       20040712
     WO 2005090298
                                             WO 2004-FI447
                           A1
                                  20050929
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
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             SN, TD, TG
     EP 1732884
                                             EP 2004-742190
                                  20061220
                           A1
            AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR
PRIORITY APPLN. INFO.:
                                              WO 2004-FI160
                                                                   A 20040319
                                                                   W 20040712
                                              WO 2004-FI447
OTHER SOURCE(S):
                          MARPAT 143:326199
GI
```

$$(CH_2)_{mN}(R?)SO_2R?$$

The invention relates to sulfonamide derivs. (shown as I; variables AΒ defined below; e.g. 2,4-dichloro-N-[4-[(4,6-dimethylpyrimidin-2yl) (methyl) amino] phenyl] benzenesulfonamide (II)). The invention also relates to the use of I as inhibitors for collagen receptor integrins, particularly $\alpha 2\beta 1$, and a process for preparing I. Methods of preparation are claimed and 37 example prepns. are included. For example, II

IT

CN

was prepared from N-(4,6-dimethylpyrimidin-2-yl)-N-methylbenzene-1,4-diamine and 2,4-dichlorobenzenesulfonyl chloride in MeCN in the presence of Et3N; the resulting mixture of mono- and bis-sulfonamide was separated by column chromatog. and the bis-sulfonamide was hydrolyzed using NaOEt/EtOH to give more monosulfonamide. For I: Rc is an (un)substituted 4-6-membered heterocyclic ring containing ≥1 N atoms, or Rc is -NR1R2, where R1 is H or alkyl, R2 is alkyl or an (un) substituted 4-6-membered heterocyclic ring containing ≥1 N atoms, or R1 and R2 taken together with the N atom to which they are attached form a heterocyclic group, which may contain ≥1 addnl. heteroatoms = O and N and which may be substituted, or R1 and R2 are absent and the N atom together with the adjacent C atom forms a heterocyclic ring, which may contain ≥1 addnl. heteroatoms = N and S and which may be substituted; RA is -(CH:CH)nQ (Q = R3- and R4-substituted naphthalen-2-yl, thien-2-yl, Ph (n = 0-1; R3 and R4 = H,halogen, aryl, alkoxy, carboxy, hydroxy, alkoxyalkyl, alkoxycarbonyl, cyano, trifluoromethyl, alkanoylamino, trifluoromethoxy, an (un) substituted aryl or heterocyclic)); m = 0, 1 (defined other than in claims); RB = H, alkyl (defined other than in claims). 686746-30-5P, 2,4-Dichloro-N-(2-methyl-1,3-benzothiazol-5yl)benzenesulfonamide 865375-73-1P, 3-Bromo-N-(2methylbenzothiazol-5-yl)benzenesulfonamide 865376-19-8P, 2,4-Dichloro-N-(2-methylthiobenzothiazol-5-yl)benzenesulfonamide RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(drug candidate; preparation of sulfonamides as inhibitors for collagen receptor integrins for treating thrombosis and cancer)

RN686746-30-5 HCAPLUS

> Benzenesulfonamide, 2,4-dichloro-N-(2-methyl-5-benzothiazolyl)- (9CI) INDEX NAME)

RN865375-73-1 HCAPLUS

Benzenesulfonamide, 3-bromo-N-(2-methyl-5-benzothiazolyl)- (9CI) CN INDEX NAME)

RN865376-19-8 HCAPLUS

Benzenesulfonamide, 2,4-dichloro-N-[2-(methylthio)-5-benzothiazolyl]-CN (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN L8

7

ACCESSION NUMBER:

2004:904114 HCAPLUS

DOCUMENT NUMBER:

141:386306

TITLE:

Color molecule-releasing compound, silver halide

photosensitive material, color filter, and manufacture

thereof

INVENTOR (S):

Makuta, Toshiyuki; Takahashi, Osamu; Mizukawa, Hiroki;

Ishiwata, Yasuhiro

PATENT ASSIGNEE(S): SOURCE:

Fuji Photo Film Co., Ltd., Japan

Jpn. Kokai Tokkyo Koho, 61 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE | |
|----|-------------------------------------|---------|-------------|--------------------------------|----------------------|-----|
| | JP 2004300331 RITY APPLN. INFO.: | A | 20041028 | JP 2003-96681 JP 2003-96681 | 20030331 20030331 | |
| AB | Disclosed is the co | lor mol | -releasing | g compound capable o | of releasing a | |
| | water-insol. color | mol. up | on the coup | oling reaction with | an oxidized | |
| | developing agent, w | herein | the compour | nd is water insol. a | at pH≤9 and | |
| | water soluble at pH | ≥10. T | he compound | d is represented by | - | |
| • | (SOL-Cp) - [L-Dye]n (| SOL-Cp | = coupler : | residue; L = divaler | it bonding group: | |
| | Dye = hydrophilic o | r oleop | hilic dve | residue: and $n = int$ | reger >1) | |
| IT | 784179-51-7 | - | | | ,eger =1,. | |
| | RL: NUU (Other use, | | | | | |
| | (color molrele | asing c | ompound in | silver halide photo | og. emulsion used | for |
| | manufacture of c | olor fi | lter) | - | 5 | |
| RN | 784179-51-7 HCAPLU | | | | | |
| CN | 2-Naphthalenecarbox | amide, | N-[[2-(acet | vlamino)phenvllmeth | vll-5-[[[[2- | |

[[cyano[5-[[3-[[(methylsulfonyl)amino]carbonyl]phenyl]sulfonyl]amino]-2benzothiazolyl] methyl] thio] phenyl] amino] carbonyl] amino] -4-[[4-[ethyl(2hydroxyethyl)amino]-2-methylphenyl]imino]-1,4-dihydro-1-oxo- (9CI) (CA INDEX NAME)

Jungan

L8 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:368925 HCAPLUS

DOCUMENT NUMBER: 140:391280

TITLE: Preparation of arylsulfonylbenzazoles as inhibitors of

11-β-hydroxy steroid dehydrogenase type 1 and

type 2.

INVENTOR(S): Vicker, Nigel; Su, Xiangdong; Ganeshapillai,

Dharshini; Purchit, Atul; Reed, Michael John; Potter,

Barry Vietor Lloyd

PATENT ASSIGNEE(S): Sterix Limited, UK SOURCE: PCT Int. Appl., 172 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND D | | ICATION NO. | DATE | | | |
|---------------|-------------|-----------------|---------------|----------------|--|--|--|
| WO 2004037251 | A1 2 | | | 20031023 | | | |
| | | AU, AZ, BA, BB, | | | | | |
| | | DK, DM, DZ, EC, | | | | | |
| | | IL, IN, IS, JP, | | | | | |
| LR, LS, | LT, LU, LV, | MA, MD, MG, MK, | MN. MW. MX. M | Z. NI. NO. NZ. | | | |
| | | RO, RU, SC, SD, | | | | | |
| | | UG, US, UZ, VC, | | | | | |
| | | MZ, SD, SL, SZ, | | | | | |
| | | TM, AT, BE, BG, | | | | | |
| FI, FR, | GB, GR, HU, | IE, IT, LU, MC, | NL, PT, RO, S | E, SI, SK, TR, | | | |
| | | CM, GA, GN, GQ, | | | | | |
| CA 2501228 | | | | | | | |
| | | | | 20031023 | | | |
| US 2004143124 | | | | 20031023 | | | |
| EP 1556040 | | | | | | | |
| | | ES, FR, GB, GR, | | | | | |
| IE, SI, | LT, LV, FI, | RO, MK, CY, AL, | TR, BG, CZ, E | E. HU. SK | | | |
| BR 2003015605 | | | | 20031023 | | | |
| CN 1723022 | A 2 | 0060118 CN 2 | 003-80105509 | 20031023 | | | |
| JP 2006514614 | | 0060511 JP 2 | 004-546183 | | | | |
| NO 2005002469 | A 2 | | | 20050523 | | | |

PRIORITY APPLN. INFO.:

GB 2002-24830 A 20021024 US 2002-436635P P 20021230

WO 2003-GB4590

W 20031023

OTHER SOURCE(S):

MARPAT 140:391280

GI

AB Title compds. [I; 1 of R1, R2 = R5SO2N(R4)L; R4 = H, hydrocarbyl; R5 = hydrocarbyl; L = optional linker group; R1R2 = atoms form a ring; X = S, O, NR6, C(R7)(R8); R6-R8 = H, hydrocarbyl], were prepared Thus, title compound (II) inhibited 11β -HSD1 with IC50 = 6.6 μ M.

IT 670272-62-5P 671200-96-7P 686746-30-5P 686746-31-6P 686746-32-7P 686746-33-8P 686746-34-9P 686746-37-2P 686746-38-3P 686746-39-4P 686746-40-7P 686746-41-8P 686746-44-1P 686746-45-2P 686746-47-4P

686746-48-5P 686746-49-6P 686746-50-9P 686746-51-0P 686746-52-1P 686746-53-2P

686746-54-3P 686746-55-4P 686746-56-5P 686746-57-6P 686746-58-7P 686746-59-8P

686746-70-3P 686746-71-4P 686746-82-7P

686746-87-2P 686747-08-0P 686747-10-4P

686747-11-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indoles, benzothiazoles, benzoxazoles, and benzimidazoles as inhibitors of hydroxy steroid dehydrogenase)

RN 670272-62-5 HCAPLUS

RN 671200-96-7 HCAPLUS

CN Benzenesulfonamide, 2,3,5,6-tetramethyl-N-(2-methyl-5-benzothiazolyl)(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \\ & \text{Me} & \\ & \text{NH} &$$

RN 686746-30-5 HCAPLUS

CN Benzenesulfonamide, 2,4-dichloro-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-31-6 HCAPLUS

CN Benzenesulfonamide, 3-chloro-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-32-7 HCAPLUS

CN Benzenesulfonamide, N-(2-methyl-5-benzothiazolyl)-4-propyl- (9CI) (CA INDEX NAME)

RN 686746-33-8 HCAPLUS

CN Benzenesulfonamide, 4-methoxy-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-34-9 HCAPLUS

CN Benzenesulfonamide, 2-chloro-6-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-37-2 HCAPLUS

CN Benzenesulfonamide, 4-bromo-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-38-3 HCAPLUS

CN [1,1'-Biphenyl]-4-sulfonamide, N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-39-4 HCAPLUS

CN Benzenesulfonamide, 2,4,6-trichloro-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-40-7 HCAPLUS

CN Benzenesulfonamide, 4-bromo-2-methyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-41-8 HCAPLUS

CN Benzamide, 3,5-dichloro-N-(2-methyl-5-benzothiazolyl)-2-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]- (9CI) (CA INDEX NAME)

RN 686746-44-1 HCAPLUS

CN Benzoic acid, 3,5-dichloro-2-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]-(9CI) (CA INDEX NAME)

RN 686746-45-2 HCAPLUS

CN Benzenesulfonamide, 2,5-dichloro-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-47-4 HCAPLUS

CN Benzenesulfonamide, 5-chloro-2-methoxy-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-48-5 HCAPLUS

CN Benzenesulfonamide, 2-cyano-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-49-6 HCAPLUS

CN Benzenesulfonamide, 2-methoxy-4-methyl-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-50-9 HCAPLUS

CN Benzenesulfonamide, 2-acetyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-51-0 HCAPLUS

CN Benzenesulfonamide, N-(2-methyl-5-benzothiazolyl)-2,4,6-tris(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 686746-52-1 HCAPLUS

CN Benzenesulfonamide, N-(2-methyl-5-benzothiazolyl)-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 686746-53-2 HCAPLUS

CN Benzoic acid, 2-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 686746-54-3, HCAPLUS

CN Benzenesulfonamide, 3,4-dimethoxy-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-55-4 HCAPLUS

CN Benzenesulfonamide, 4-methoxy-2,3,5,6-tetramethyl-N-(2-methyl-5-benzothiazolyl)- (9CI) (CA INDEX NAME)

RN 686746-56-5 HCAPLUS

CN Benzenesulfonamide, 4-(1,1-dimethylethyl)-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-57-6 HCAPLUS

CN Benzenesulfonamide, 2,3,4,5,6-pentamethyl-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-58-7 HCAPLUS

CN Acetamide, N-[4-[[(2-methyl-5-benzothiazolyl)amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 686746-59-8 HCAPLUS

CN Benzenesulfonamide, 2,3,4,5,6-pentafluoro-N-(2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-70-3 HCAPLUS

CN Benzenesulfonamide, 2,5-dichloro-N-(4-chloro-2-methyl-5-benzothiazolyl)-(9CI) (CA INDEX NAME)

RN 686746-71-4 HCAPLUS

CN Benzenesulfonamide, N-(4-chloro-2-methyl-5-benzothiazolyl)-4-propyl- (9CI) (CA INDEX NAME)

RN 686746-82-7 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-(4-chloro-2-methyl-5-benzothiazolyl)-2-methyl-(9CI) (CA:INDEX NAME)

RN 686746-87-2 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-(4,6-dichloro-2-methyl-5-benzothiazolyl)-2-methyl- (9CI) (CA INDEX NAME)

RN686747-08-0 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-(2-chloro-5-benzothiazoly1)-2-methy1- (9CI) (CA INDEX NAME)

RN686747-10-4 HCAPLUS

Benzenesulfonamide, 3-chloro-2-methyl-N-[2-(methylamino)-5-benzothiazolyl]-CN (9CI) (CA INDEX NAME)

RN686747-11-5 HCAPLUS

Benzenesulfonamide, 3-chloro-N-[2-(diethylamino)-5-benzothiazolyl]-2-CN methyl- (9CI) (CA INDEX NAME)

ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:686578 HCAPLUS

DOCUMENT NUMBER: 133:259388

TITLE: Heat development photosensitive material for printing

platemaking

INVENTOR (S): Ezoe, Toshihide; Taniguchi, Masahiko PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan SOURCE:

Jpn. Kokai Tokkyo Koho, 57 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

03/13/2007

Page 39

GI

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|----------|
| | | | | |
| JP 2000267222 | Α | 20000929 | JP 1999-73951 | 19990318 |
| PRIORITY APPLN. INFO.: | | | JP 1999-73951 | 19990318 |
| OTHER SOURCE(S): | MARPAT | 133:259388 | | |

$$R^1$$
 R^2
 R^3
 R^4
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 R^9
 R^9
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 R^9
 R^9
 R^9

AB The title photosensitive material, containing a photosensitive Ag halide, a reducible Ag salt, a reducing agent, a binder, a nucleating agent, and a phenolic compound I or II [R1-3, R6-9, X1, X2 = H, halo, substituent linking to the benzene ring by C, O, N, S or P atom, ≥1 of X1 and X2 is NR4R5; R4, R5, R10. R11 = H, alkyl, alkenyl, alkynyl, aryl, heterocyclic group, COR, COCOR, SO2R, SOR, POR2, C(:NR')R; R, R' = H, alkyl, aryl, heterocyclic group, amino, alkoxy, aryloxy (the adjacent groups in these groups may link each other to form a ring)] on ≥1 side of the same surfaces of a support, contains ≥1 selected from a compound X1JnB1 (X1 = residue of a photog. inhibitor having a N-containing heterocycle; J = divalent linking group; B1 = ballast; n ≥ 1), a polymer having a repeating unit derived from a monomer QX2 (Q = ethylenic unsatd. group, ethylenic unsatd. group- containing group; X2 = residue of photog. inhibitor having a N-containing heterocycle), and compound A1X3 (A1 = water-soluble group-containing group; X3 = residue of a photog. inhibitor having a N-containing

heterocycle). The material shows super-high contrast and little variation in Dmax upon storage and is suited for photomech. process. 212572-28-6

RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)

(photothermog. material containing development inhibitor and phenolic compound development accelerator)

RN 212572-28-6 HCAPLUS

CN 2-Propenoic acid, butyl ester, polymer with N-(2,3-dihydro-2-thioxo-5-benzothiazolyl)-4-ethenylbenzenesulfonamide (9CI) (CA INDEX NAME)

CM 1

TΤ

CRN 212572-27-5 CMF C15 H12 N2 O2 S3

CM 2

CRN 141-32-2 CMF C7 H12 O2

ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1998:555880 HCAPLUS

DOCUMENT NUMBER:

129:237713

TITLE:

Thermographic black and white photographic material

with high contrast and fog resistance and

image-forming method using it

INVENTOR(S):

Yamada, Taketoshi; Komamura, Tawara

PATENT ASSIGNEE(S):

Konica Co., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 31 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE: Japanese FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|----------|--------------|-----------------|----------|
| | - | | | |
| JP 10228077 | Α | 19980825 | JP 1997-31939 | 19970217 |
| PRIORITY APPLN. INFO.: | | | JP 1997-31939 | 19970217 |
| AR The material conta | ina at ' | 1000+ 0 6400 | | |

AB The material contains at least a binder, a Ag halide, an organic Ag salt, a hydrazine derivative, and one of the following compds. (1) X1JnB (X1 = residue of a photog. fog inhibitor with N-containing heterocyclic ring; J = bivalent linking group; B = ballast group; n ≥1); (2) a polymer containing QX2 (Q = ethylenically unsatd. group; group having an ethylenically unsatd. group; $X^2 = X^1$); (3) AX3 (A = water-soluble group; $X^3 = X^1$). A black and white image is formed by developing the material for 1-180 s. The material shows high contrast, improved storage stability for a long time, and less fogging of an unexposed area after development.

IT 212572-28-6

> RL: TEM (Technical or engineered material use); USES (Uses) (fog inhibitor; thermog. black and white organic silver salt photog. material containing fog inhibitor)

212572-28-6 HCAPLUS RN

CN 2-Propenoic acid, butyl ester, polymer with N-(2,3-dihydro-2-thioxo-5benzothiazolyl)-4-ethenylbenzenesulfonamide (9CI) (CA INDEX NAME)

CM 1

CRN 212572-27-5 CMF C15 H12 N2 O2 S3

CM 2

CRN 141-32-2 CMF C7 H12 O2

ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN L8

ACCESSION NUMBER: 1962:469757 HCAPLUS

DOCUMENT NUMBER: 57:69757

ORIGINAL REFERENCE NO.: 57:13924f-i,13925a-f

Azomethine dyes. IV. Indoaniline dyes derived from TITLE:

heterocyclic N-substituted 1-hydroxy-2-naphthamides AUTHOR (S):

Portnaya, B. S.; Bobkova, T. P.; Krasheninnikova, M.

V.; Chel'tsov, V. S.; Levkoev, I. I.

SOURCE: Ts. Vses. Nauchn.-Issled. Kinofotoinst. (1960), (No.

40), 106-18

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

For diagram(s), see printed CA Issue. cf. CA 51, 5022i; 52, 15505e. N-Thiazolyl- and -benzothiazolyl derivs. of 1-hydroxy-2-naphthamide (Ia) were prepared and converted to indoanillne dyes. A mixture of 4.08 g. p-MeC6H4SO2Cl, 3.28 g. 2-methyl-5aminobenzothiazole, and 16 ml. C5H5N heated 90 min. on a steam bath, cooled, and treated with 200 ml. H2O and 25 ml. concentrated HCl gave 5.2 g. (91%) of 2-methyl5-p-toluenesulfonamidobenzothiazole (I), m. 172-30 (alc.). A solution of 12.75 g. I and 3.2 g. KOH in 80 ml. H2O stirred 30 min. with 10.08 g. Me2SO4, and 30 min. with 1.6 g. NaOH in 40 ml. H2O gave 9.1 g. (68%) N-methyl derivative (II) of I, m. 110-11° (alc.). Refluxing 10 g. II with 120 ml. concentrated HCl 2 hrs., adding 600 ml. H2O, neutralizing with 30% NaOH, extracting with Et20, and evaporating gave 63.5% 2-methyl-5-(N-methylamino)benzothiazole (III), m. 77-80 (petr. ether). Addition of 7.7 g. stearoyl chloride to 4.34 g. 2,5-Br(O2N)C6H3NH2 and 20 ml. C5H5N, refluxing 1 hr., pouring into 80 g. ice and 25 ml. HCl, washing with H2O, Me2CO, and Et2O gave 71% 2,5-Br(O2N)C6H3NHCOC17H35 (IV), m. 115-160 (alc.). Na2S (4.16 g.) in 25 ml. 50% alc. was added to 4.8 g. IV in 40 ml. alc., refluxed 1.5 hrs., filtered, diluted with 400 ml. H2O, refiltered, heated 30 min. with 40 ml. concentrated HCl to a crude product.

The

yellow crystals refluxed with 50 ml. 20% HCl and 12 ml. alc. 2 hrs., filtered, extracted with Et20, the extract washed with 2% NaOH and H2O, evaporated,

2-heptadecyl-5-nitrobenzothiazole (V), yellow crystals, m. 57-8° (alc.). Reduction of 4.18 g. V in 32 ml. refluxing alc. with 13.5 g. SnCl2 and 20 ml. concentrated HCl, filtered, basified with 40% NaOH, extracted with Et20, evaporated and recrystd. from alc. gave 74% 2-heptadecyl-5-aminobenzothiazole (VI), m. 67-8°, N-(p-toluenesulfonyl) derivative (VII), 89% light yellow crystals, m.p. 77-80 (MeOH), N-methyl-VII (VIII), 68% light yellow crystals, m. 61-20 (MeOH). Hydrolysis of VIII gave 70% of 1-heptadecyl-5methylaminobenzothiazole (IX), m. 42° (alc.). Equimolar amts. of 1,2-HOC10H6CO2Ph and the appropriate amine were heated in vacuo at 135-70°, washed with H2O and 5% NaHCO3, and recrystd. from alc. to give N-substituted derivs. of Ia (substituent, % yield, m.p.): 2-thiazolyl, 40, 230-1°; 4,5-dicarbethoxy-2-thiazolyl, 85, 239-40°; 2benzothiazolyl (X), 60, 244-5°; 5,6-dicarbethoxy-2-benzothiazolyl, 80, 258-6°; 2-methyl-5benzothiazolyl, 80, 234-5°; 2-methyl-6-benzothiazolyl, 63, 253-4°; 2-heptadecyl5-benzothiazolyl (XI), 94, 149°. XI (1.05 g.) and 3.75 ml. concentrated H2SO4 shaken 1 hr. at 30-5°, 1 hr. at 40-5°, the viscous mass added to 4 g. NaCl and 10 g. ice, filtered, and washed with 15% NaCl gave 54% N-(2-heptadecyl-5-benzothiazolyl)-1hydroxy-4-sulfo-2-naphthamide, m. 249-500 (alc.). A solution of 2.01 g. IX in 5 ml. C6H6 stirred with 1.03 g. 1,2-HOC10H6COCl and 1 ml. PhNMe2 in 7 ml. C6H6 for 6 hrs., extracted with 20 ml. Et2O, washed with 5% HCl, 3% Na2CO3, and H2O, dried over Na2SO4, evaporated, recrystd. from alc. and twice from MeOH gave 46% N-methyl-N(2-heptadecyl-5-benzothiazolyl)-1-hydroxy-2naphthamide, m.p. 52-30; 4-sulfoderiv., 25%, m. 183-5° (3 times from MeOH). Condensation of the amides with 4-Et2NC6H4NH2 and ZnCl2 in alc. gave indoaniline dyes which were chromatographed in C6H6 or CHCl3 solution through Al203. The following derivs. of XII were obtained (R, R', recrystn. solvent, color, % yield, m.p., λmaximum in MeOH, alc., gelatin in mµ): H, 2-thiazolyl, PrOH, green, 25, 184-5°, 708, -, 680; H, 4,5-dicarbethoxy-2-thiazolyl, PrOH, bronze, 25, 165-6°, 729, -, -; H, 2-benzothiazolyl, PrOH, bronze needles, 15, 188°, 721, 722-4°, 690; H, 4, 5-dicarbethoxy-2-benzothiazolyl, BuOH, green prisms, 12, 202-3°, -, 728, -; H, 2-methyl-5-benzothiazolyl, BuOH, green prisms, 87, 206-7°, 694, -, 670; Me, 2-methyl-5-benzothiazolyl, MeOH, blue prisms, 11, 160-2°, 645, -, 605; H, 2-methyl-6-benzothiazolyl, PrOH, blue needles, 89, 199-200°, 698, -, 590; H, H -, -, -, 692, 690, 680; H, 2-heptadecyl-5-benzothiazolyl, -, -, -, -, -, 690; Me, 2-heptadecyl-5-benzothiazolyl, -, -, -, -, -, 640. The absorption spectra in gelatin are given. 93733-28-9P, p-Toluenesulfonamide, N-(2-methyl-5-benzothiazolyl)-96774-24-2P, p-Toluenesulfonamide, N-(2-heptadecyl-5benzothiazolyl) -RL: PREP (Preparation) (preparation of) RN93733-28-9 HCAPLUS CNp-Toluenesulfonamide, N-(2-methyl-5-benzothiazolyl)- (7CI) (CA INDEX NAME)

and the residue chromatographed in C66 through Al2O3 gave 55% of

RN 96774-24-2 HCAPLUS

CN p-Toluenesulfonamide, N-(2-heptadecyl-5-benzothiazolyl)- (7CI) (CA INDEX NAME)

=> d l15 ibib abs hitstr 1-15

L15 ANSWER 1 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2003:150554 HCAPLUS

DOCUMENT NUMBER:

138:188073

TITLE:

Preparation of dipeptide heterocyclic aromatic

compounds as growth hormone secretagogues

INVENTOR(S):

Tino, Joseph A.

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA

SOURCE:

U.S., 157 pp., Cont.-in-part of U.S. Ser. No. 506,749,

abandoned.
CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|------------------------|------|----------|-----------------|----|------------|
| | | | | | |
| US 6525203 | B1 | 20030225 | US 2000-662448 | | 20000914 < |
| US 6518292 | B1 | 20030211 | US 2000-506749 | | 20000218 < |
| ZA 2001006854 | A | 20021120 | ZA 2001-6854 | | 20010820 < |
| US 6660760 | B1 | 20031209 | US 2002-282182 | | 20021028 < |
| US 2004002525 | A1 | 20040101 | US 2002-281818 | | 20021028 < |
| US 6969727 | B2 | 20051129 | | | |
| US 2004029935 | A1 | 20040212 | US 2002-281649 | | 20021028 < |
| US 6908938 | B2 | 20050621 | | | |
| US 2004072881 | A1 | 20040415 | US 2002-281848 | | 20021028 < |
| US 7053110 | B2 | 20060530 | | | |
| PRIORITY APPLN. INFO.: | | | US 1999-124131P | P | 19990312 |
| | | | US 1999-154919P | P | 19990921 |
| | | | US 2000-506749 | A2 | 20000218 |
| | | | | | |

OTHER SOURCE(S):

MARPAT 138:188073

GΙ

AB R1R1aCXaNR6COYXb [R1 = (un)substituted alkyl, (hetero)aryl(alkyl), etc.; Rla = H or (cyclo)alkyl; R6 = H, (cyclo)alkyl, alkenyl, aryl; Xa = substituted 2-benzoxazolyl, 2-benzothiazolyl, or 2-benzimidazolyl; Xb = (di) (alkyl) amino, (un) substituted imidazolyl; Y = phenylene, (phenylene-interrupted) alkylene, (un) substituted alkylene, aza- or oxaalkylene, or alkenylene] were prepared as growth hormone production and/or release stimulants. Thus, dipeptide benzimidazole derivative I (Boc = tert-butoxycarbonyl) was prepared by a multistep procedure starting from Boc-D-Ser(CH2Ph)-OH, 4-nitro-o-phenylenediamine, Boc-methylalanine, and MeSO2Cl.

IT 295335-10-3P

> RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of dipeptide heterocyclic aromatic compds. as growth hormone secretagogues)

RN 295335-10-3 HCAPLUS

Propanamide, 2-amino-2-methyl-N-[(1S)-2-(phenylmethoxy)-1-[5-CN [(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

2002:814232 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 137:326555

TITLE: Azo dye-containing coloring composition for image

formation with improved ozone resistance

INVENTOR(S): Fujiwara, Toshiki; Hanaki, Naoyuki; Tanaka, Shiqeaki;

Omatsu, Tadashi; Yabuki, Yoshiharu Fuji Photo Film Co., Ltd., Japan

PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 256 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|------------|
| | | | | |
| WO 2002083795 | A2 | 20021024 | WO 2002-JP3490 | 20020408 < |
| WO 2002083795 | A3 | 20030306 | | |

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              LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
              PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
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PRIORITY APPLN. INFO.:
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                                                                     20010409
                                             JP 2001-110334
                                                                  A 20010409
                                             JP 2001-110335
                                                                  Α
                                                                     20010409
                                             JP 2001-110457
                                                                  Α
                                                                     20010409 -
                                             JP 2001-237903
                                                                  Α
                                                                     20010806
                                             JP 2001-254878
                                                                  Α
                                                                     20010824
                                             JP 2002-12015
                                                                  Α
                                                                     20020121
                                             WO 2002-JP3490
                                                                  W
                                                                     20020408
OTHER SOURCE(S):
                         MARPAT 137:326555
     A coloring composition for image formation comprises an azo dye having an
aromatic
     nitrogen-containing 6-membered heterocyclic ring as a coupling component and
     which comprises an azo compound having an oxidation potential better than 1.0 V
     vs.SCE and having at least two substituents having a pKa value of -10 to 5
     in water. Improved ozone resistance is obtained with an azo compound
     showing a maximum absorption at a wavelength between 500 nm and 580 nm with a
     half-value width of 150 nm or narrower. The dyes may be used in jet ink
     compns., color filters, color toners, etc. In an example,
     2-\overline{\text{amino-4}}, 5-\overline{\text{dicyano-1-}} (ethoxycarbonylmethyl) imidazole\rightarrow 2, 6-\overline{\text{constant}}
     bis(octylanilino)-4-methylpyridine was prepared as an azo dye (λmax
     528 nm in DMF).
IT
     473465-65-5 473555-05-4
     RL: TEM (Technical or engineered material use); USES (Uses)
        (dye; azo dye-containing coloring compns. for image formation with improved
        ozone resistance)
RN
     473465-65-5 HCAPLUS
     Benzenesulfonamide, N-[2-[[5-[[4-cyano-3-(1,1-dimethylethyl)-1-(5-nitro-2-
CN
     benzothiazolyl)-1H-pyrazol-5-yl]azo]-4-methyl-6-[(1,1,3,3-
     tetramethylbutyl)amino]-2-pyridinyl](4-octylphenyl)amino]-6-
     benzothiazolyl]-2-(octyloxy)-5-(1,1,3,3-tetramethylbutoxy)- (9CI) (CA
     INDEX NAME)
```

PAGE 1-A

PAGE 1-B

Bu-t

RN 473555-05-4 HCAPLUS

CN Benzenesulfonamide, 2-(octyloxy)-N-[2-[[5-[(3-phenyl-1,2,4-thiadiazol-5-yl)azo]-6-[(1,1,3,3-tetramethylbutyl)amino]-2-pyridinyl](2,4,6-trimethylphenyl)amino]-6-benzothiazolyl]-4-(1,1,3,3-tetramethylbutyl)-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{PAGE 1-A} \\ \text{Me} - (\text{CH}_2)_{7-0} \\ \text{Me} \\ \text{Me} \\ \text{Me} \end{array}$$

- Ph

- CMe₃

L15 ANSWER 3 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:814122 HCAPLUS

DOCUMENT NUMBER: 137:326554

TITLE: Pyrazole azo dyes, their production and coupling

agents therefor

INVENTOR(S): Fujiwara, Toshiki; Hanaki, Naoyuki; Tanaka, Shigeaki;

Omatsu, Tadashi; Yabuki, Yoshiharu Fuji Photo Film Co., Ltd., Japan

PATENT ASSIGNEE(S): SOURCE: PCT Int. Appl., 137 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| P. | PATENT NO. KIND | | | | | | DATE | | ; | APPL | ICAT | | DATE | | | | |
|---------|-----------------|--|---|---|---|---|--|---|--|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| | O 200: | | | | | | 2002 | | | WO 2 | 002- | JP34: | | 20020408 < | | | |
| | W: | AE, CO, GM, LT, PT, UG, | AG, CR, HR, LU, RO, US, GM, | AL, CU, HU, LV, RU, UZ, KE, | AM, CZ, ID, MA, SD, VN, LS, | AT, DE, IL, MD, SE, YU, MW, | AU, DK, IN, MG, SG, ZA, | AZ, DM, IS, MK, SI, ZM, SD, | BA, DZ, KE, MN, SK, ZW SL, | EC, KG, MW, SL, | EE, KP, MX, TJ, | ES, KR, MZ, TM, | FI, KZ, NO, TN, | GB, LC, NZ, TR, | GD, LK, OM, TT, | GE, LR, PH, TZ, | GH, LS, PL, UA, |
| _ | | BF, | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, | TG |
| J | P 200 | 23221 | 51 | | Α | | 2002 | 1108 | | JP 2 | 001- | 1262 | 39 | | 2 | 0010 | 424 < |
| J | P 200 | 23710 | 79 | | Α | | 2002 | 1226 | | JP 2 | 002- | 1210 | 8 | | 2 | 0020 | 121 < |
| E | P 137 | 7640 | | | A2 | | 2004 | 0107 | : | EP 2 | 002- | 7087 | 77 | | 2 | 020 | 108 |
| | R: | AT, IE, | | | | | ES, RO, | | | | | LI, | LU, | NL, | SE, | MC, | PT, |
| C | N 150 | 1962 | | | Α | | 2004 | 0602 | | CN 2 | 002- | 8080 | 09 | • | 2 | 0020 | 108 |
| | S 200 S 710 | | | | | | 2004 2006 | | | JS 2 | 003-4 | 4734 | 19 | | 2 | 0030 | 930 < |
| PRIORI | TY AP | PLN. | INFO | . : | | | | | | TP 2 | 001- | 1104 | 58 | | À 2 | 00104 | 109 |
| | | | | | | | | | | | | 1262 | | | A 2 | | |
| | | | | | | | | | | | | 1210 | | | A 2 | | |
| | | | | | | | | | | | | JP34: | _ | | - | | |
| OTHER : | SOURC | E(S): | | | MAR | PAT | 137: | 3265 | | | | | | , | . 2 | | |

$$\begin{array}{c|c}
R^1 & R^2 \\
N & A^{1-A^2} \\
N = N & NR^{4}R^5 \\
R^3 & NR^{6}R^7 & I
\end{array}$$

Aminopyrazole diazo component-based azo dyes (I; A1, A2 = N, optionally substituted -CH=; R1 = H, organic group; R2 = H, halogen, CN; R3 = H, organic group; R4, R5, R6, R7 = H, organic group, carboxy, sulfo, carbamoyl) are obtained from novel diamino heterocyclic coupling components. I are suitable for image formation and recording and have excellent ozone resistance. In an example, 5-amino-3-tert-butyl-4-cyanopyrazole was diazotized and coupled with 3-cyano-4-methyl-2,6-bis(p-octylanilino)pyridine and the product was condensed with 2-chlorobenzothiazole to give a dye (λmax 545 nm in DMF).

IT 473465-24-6P 473465-65-5P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(dye; production of pyrazole azo dyes for image formation and recording) 473465-24-6 HCAPLUS

RN 473465-24-6 HCAPLUS

CN Benzenesulfonamide, N-[2-[4-cyano-5-[[5-cyano-4-methyl-6-[(1,1,3,3-tetramethylbutyl)amino]-2-[(2,4,6-trimethylphenyl)amino]-3-pyridinyl]azo]-3-(1,1-dimethylethyl)-1H-pyrazol-1-yl]-6-benzothiazolyl]-2-(octyloxy)-5-(1,1,3,3-tetramethylbutyl)- (9CI) (CA INDEX NAME)

RN 473465-65-5 HCAPLUS

CN Benzenesulfonamide, N-[2-[[5-[[4-cyano-3-(1,1-dimethylethyl)-1-(5-nitro-2-benzothiazolyl)-1H-pyrazol-5-yl]azo]-4-methyl-6-[(1,1,3,3-tetramethylbutyl)amino]-2-pyridinyl](4-octylphenyl)amino]-6-benzothiazolyl]-2-(octyloxy)-5-(1,1,3,3-tetramethylbutoxy)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

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L15 ANSWER 4 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2002:353428 HCAPLUS

DOCUMENT NUMBER:

136:369603

TITLE:

Preparation of (sulfonylamino) (aminomethylidene) indoli

nones as cell proliferation inhibitors.

INVENTOR(S):

Walter, Rainer; Heckel, Armin; Roth, Gerald Juergen; Kley, Joerg; Schnapp, Gisela; Lenter, Martin; Van Meel, Jacobus Constantinus Antonius; Spevak, Walter;

Weyer-Czernilofsky, Ulrike

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma K.-G., Germany

SOURCE:

PCT Int. Appl., 112 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent German

LANGUAGE:

GETII

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT : | | KIND DATE | | 1 | APPL | ICAT: | ION I | | DATE | | | | | | | | |
|----------|-----|-----------|-----|-----------|------|-------|-------|-----|------|------|-----|------------|-----|-----|-----|-----|--|
| | | | | | | | | | | | | | | | | | |
| | | | | A1 | : | 2002 | 0510 | 1 | WO 2 | 001- | | 20011030 < | | | | | |
| W: | ΑE, | AG, | AL, | AM, | AT, | AU, | ΑZ, | BA, | BB, | BG, | BR, | BY, | ΒZ, | CA, | CH, | CN, | |
| | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | ES, | FI, | GB, | GD, | GE, | GH, | |
| | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KP, | KR, | KZ, | LC, | LK, | LR, | |
| | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NO, | NZ, | PH, | PL, | |
| | PT, | RO, | RU, | SD, | SE, | SG, | SI, | SK, | SL, | TJ, | TM, | TR, | TT, | TZ, | UA, | UG, | |

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             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     DE 10054019
                          A1
                                 20020523
                                             DE 2000-10054019
                                                                     20001101 <--
     AU 200215980
                          Α
                                 20020515
                                             AU 2002-15980
                                                                     20011030 <--
     EP 1341760
                                 20030910
                          A1
                                             EP 2001-992699
                                                                     20011030
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2004513113
                          Т
                                 20040430
                                             JP 2002-539324
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     US 2003069299
                          A1
                                 20030410
                                             US 2001-2939
                                                                     20011101 <--
     US 6638965
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                                 20031028
     US 2004044222
                          A1
                                 20040304
                                             US 2003-646423
                                                                     20030822 <--
     US 7160901
                          B2
                                 20070109
     US 2004044053
                          A1
                                 20040304
                                             US 2003-646495
                                                                     20030822 <--
     US 7166615
                          B2
                                 20070123
PRIORITY APPLN. INFO.:
                                                                     20001101
                                             DE 2000-10054019
                                                                  Α
                                             US 2000-251055P
                                                                  Р
                                                                     20001201
                                             WO 2001-EP12523
                                                                  W
                                                                     20011030
                                                                  A3 20011101
                                             US 2001-2939
```

OTHER SOURCE(S):

MARPAT 136:369603

GI

$$R^{2}SO_{2}NR^{6}$$
 $NR^{4}R^{5}$
 $NR^{4}R^{5}$
 $NR^{4}R^{5}$

Title compds. [I; X = O, S; R1 = H, alkoxycarbonyl, alkanoyl; R2 = AB (substituted) alkyl, alkenyl, Ph, heteroaryl, cycloalkyl, naphthyl, etc.; R3 = H, alkyl; R4 = (substituted) Ph, naphthyl, heteroaryl; R5, R6 = H, alkyl], were prepared Thus, 1-acetyl-3-(1-ethoxy-1-phenylmethylidene)-5-(Nacetyl-N-phenylsulfonylamino)-2-indolinone (preparation given) and 4-[N-acetyl-N-(2-trifluoracetylaminoethyl)amino]aniline (preparation given) were heated in DMF for 6 h at 120° to give 49% (Z)-3-[1-[4-[Nacetyl-N-(2-aminoethyl)amino]phenylamino]-1-phenylmethylidene]-5phenylsulfonylamino-2-indolinone. Tested I inhibited proliferation of leiomyosarcoma SK-UT-1B cells in mice at <0.01 μ M-1.0 μ M. IT 422518-12-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (sulfonylamino) (aminomethylidene) indolinones as cell proliferation inhibitors)

RN422518-12-5 HCAPLUS

CN2H-Indol-2-one, 1-acetyl-1,3-dihydro-5-[(phenylsulfonyl)amino]- (9CI) INDEX NAME)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

3

ACCESSION NUMBER:

2002:31423 HCAPLUS

DOCUMENT NUMBER:

136:102388

TITLE:

Preparation of 2-(benzoazolidinylene)propane-1,3-dione

derivatives as GnRH receptor antagonists

INVENTOR (S):

Hirano, Masaaki; Kawaminami, Eiji; Toyoshima, Akira; Moritomo, Hiroyuki; Seki, Norio; Wakayama, Ryutaro;

Okada, Minoru; Kusayama, Toshiyuki

PATENT ASSIGNEE(S):

Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE:

PCT Int. Appl., 70 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| | | | APPLICATION NO. | | | | |
|------------|----------------|-------------------|----------------------|------------------|--|--|--|
| | 002002533 | A1 20020110 | WO 2001-JP5813 | | | | |
| | W: AE, AG, AI | , AM, AT, AU, AZ, | BA, BB, BG, BR, BY, | BZ, CA, CH, CN, | | | |
| | CO, CR, CU | , CZ, DE, DK, DM, | DZ, EC, EE, ES, FI, | GB, GD, GE, GH, | | | |
| | | | JP, KE, KG, KR, KZ, | | | | |
| | | | MN, MW, MX, MZ, NO, | | | | |
| | | | TJ, TM, TR, TT, TZ, | | | | |
| | VN, YU, ZA | | | | | | |
| I | RW: GH, GM, KE | , LS, MW, MZ, SD, | SL, SZ, TZ, UG, ZW, | AT, BE, CH, CY, | | | |
| | | | IE, IT, LU, MC, NL, | | | | |
| | | | GW, ML, MR, NE, SN, | | | | |
| CA 24 | | | CA 2001-2415010 | | | | |
| AU 20 | 00171022 | A 20020114 | AU 2001-71022 | 20010704 < | | | |
| | | | EP 2001-949914 | | | | |
| | | B1 20060405 | | 20010701 | | | |
| | | | GB, GR, IT, LI, LU, | NI. SE MC PT | | | |
| | | , LV, FI, RO, MK, | | ND, 02, 110, 11, | | | |
| AT 32 | 22485 | T 20060415 | AT 2001-949914 | 20010704 | | | |
| | 300398 | Т 20060731 | PT 2001-949914 | 20010704 | | | |
| ES 22 | 261437 | T3 20061116 | ES 2001-1949914 | 20010704 | | | |
| | 003191164 | A1 20031110 | US 2002-311688 | 20010704 | | | |
| | | B2 20051101 | | 20021219 | | | |
| | | | US 2005-155595 | 20050620 < | | | |
| | APPLN. INFO.: | A1 20051201 | JP 2000-204425 | | | | |
| | million. | | JP 2001-153372 | | | | |
| | | | WO 2001-153372 | | | | |
| | | • | | | | | |
| OTHER SOUR | RCE(S): | MARPAT 136:1023 | US 2002-311688 88 | A3 20021219 | | | |

AB Described are medicinal compns., in particular, gonadotropin releasing hormone (GnRH) receptor antagonists comprising propane-1,3-dione derivs. represented by the following general formula [I; R1 , R2, R3, R4 = H, NO2, cyano, halo, (un) substituted hydrocarbyl, heterocyclyl, OH, CO2H, acyloxy, or acyl, substituent-S(0)n, H-S(0)n (wherein n = an integer of 0-2), (un) substituted CONH2, SO2NH2, or NH2; or two adjacent groups selected from R1-R4 are taken together to form aryl or cycloalkenyl; R5, R6 = H, halo, (un) substituted hydrocarbyl or NH2; X1, X2 = N, S, O; A, B = (un) substituted aryl or heterocyclyl; Z1, Z2, Z3, Z4 = C, N; provided that (1) when X1 and X2 are S or O, both or one of R5 and R6 is absent or (2) when 1 to 4 of Z1, Z2, Z3, and /or Z4 is N, the corresponding R1, R2, R3, and/or R4 is absent.] as the active ingredient. These compds. I are nonpeptide compds. having a GnRH antagonism and lowering sex hormone and are useful for the treatment of sex hormone-dependent diseases such as prostate cancer, breast cancer, endometriosis, and hysteromyoma. Thus, K2CO3 and NaI were successively added to a son. of 1-(3,5-difluorophenyl)-2-(5-hydroxy-1,3-dihydro-2H-benzimidazol-2-ylidene)-3-phenylpropane-1,3dione (preparation given) and 3-chloromethylpyridine hydrochloride in MeCN and stirred at 80° for 3.5 h to give 1-(3,5-difluorophenyl)-2-[5-(3pyridylmethoxy) -1,3-dihydro-2H-benzimidazol-2-ylidene]-3-phenylpropane-1,3dione (II). II and 24 other compds. I in vitro showed IC50 of 10-10 to 10-9 M for inhibiting the binding of 125I-D-Trp6-LHRH to human GnRH receptor. In particular, 2-(dihydrobenzoimidazol-2-ylidene)propane-1,3dione derivs. exhibited the GnRH receptor-inhibitory activity equivalent to that of the peptide GnRH antagonist cetrorelix.

IT 388596-43-8P 388596-44-9P 388596-45-0P 388596-46-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (benzoazolidinylene)propanedione derivs. as GnRH receptor antagonists for treating sex hormone-dependent diseases) 388596-43-8 HCAPLUS

Acetamide, N-[4-[[[2-[1-benzoyl-2-(3,5-difluorophenyl)-2-oxoethylidene]-2,3-dihydro-1H-benzimidazol-5-yl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

RN CN

RN 388596-44-9 HCAPLUS

CN Benzenesulfonamide, N-[2-[1-(3,5-difluorobenzoyl)-2-(3-methylphenyl)-2-oxoethylidene]-2,3-dihydro-1H-benzimidazol-5-yl]-4-fluoro-(9CI) (CA INDEX NAME)

RN 388596-45-0 HCAPLUS

CN Benzenesulfonamide, N-[2-[1-(3,5-difluorobenzoyl)-2-(4-fluorophenyl)-2-oxoethylidene]-2,3-dihydro-1H-benzimidazol-5-yl]-4-methoxy- (9CI) (CA INDEX NAME)

RN 388596-46-1 HCAPLUS

CN Benzenesulfonamide, N-[2-[1-(3,5-difluorobenzoyl)-2-(2-methoxyphenyl)-2-oxoethylidene]-2,3-dihydro-1H-benzimidazol-5-yl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

$$F_{3}C$$

$$S = NH$$

$$MeO$$

$$MeO$$

IT 388600-59-7, N-[2-[1-Benzoyl-2-(3,5-difluorophenyl)-2-

oxoethylidene]-2,3-dihydro-1H-benzimidazol-5-yl]-4-

methylbenzenesulfonamide

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of (benzoazolidinylene) propanedione derivs. as GnRH receptor antagonists for treating sex hormone-dependent diseases)

RN388600-59-7 HCAPLUS

CN Benzenesulfonamide, N-[2-[1-benzoyl-2-(3,5-difluorophenyl)-2oxoethylidene] -2,3-dihydro-1H-benzimidazol-5-yl] -4-methyl- (9CI) INDEX NAME)

REFERENCE COUNT:

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2001:581738 HCAPLUS

DOCUMENT NUMBER:

135:175421

TITLE:

Integrin expression inhibitors

INVENTOR(S):

Wakabayashi, Toshiaki; Funahashi, Yasuhiro; Hata, Naoko; Semba, Taro; Yamamoto, Yuji; Haneda, Toru; Owa, Takashi; Tsuruoka, Akihiko; Kamata, Junichi; Okabe, Tadashi; Takahashi, Keiko; Nara, Kazumasa; Hamaoka,

Shinichi; Ueda, Norihiro

PATENT ASSIGNEE(S): SOURCE:

Eisai Co., Ltd., Japan PCT Int. Appl., 153 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ----

| WO | 20010 | 5660 | 7 | | A1 | 2 | 2001 | 0809 | W | 0 2 | 001- | : | 20010201 < | | | | | |
|----------|-------|-------|------|------------|-----|-----|------|------|-----|------|-------|-------|------------|-----|------|-------|-----|-------|
| | W: | AU, | CA, | CN, | HŲ, | JP, | KR, | MX, | NO, | NZ, | RU, | | | | | | | |
| | RW: | ΑT, | BE, | CH, | CY, | DE, | DK, | ES, | FI, | FR, | GB, | GR, | ΙE, | IT, | LU | MC, | NL, | , |
| | | PT, | SE, | TR | | | | | | | | | | | | | | |
| CA | 23990 | 001 | | | A1 | 2 | 2001 | 0809 | C | A 2 | 001-2 | 23990 | 001 | | : | 20010 | 201 | < |
| AU | 20010 | 2886 | 57 | | A5 | 2 | 2001 | 0814 | Α | .U 2 | 001-2 | 2886 | 7 | | | 20010 | 201 | < |
| AU | 78150 | 06 | | | B2 | 2 | 2005 | 0526 | | | | | | | | | | |
| EP | 12582 | 252 | | | A1 | 2 | 2002 | 1120 | E | P 2 | 001-9 | 94894 | 41 | | | 20010 | 201 | < |
| | R: | ΑT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR, | IT, | LI, | LU, | NL, | SE | MC, | PT, | , 330 |
| | | | FI, | | | | | | | | | | | | | | | |
| HU | 20030 | 0544 | 1 | | A2 | 2 | 2003 | 0728 | H | U 2 | 003-5 | 544 | | | : | 20010 | 201 | |
| NZ | 52029 | 99 | | | Α | 2 | 2004 | 0528 | N | Z 2 | 001-5 | 5202 | 99 | | : | 20010 | 201 | |
| RU | 22408 | 326 | | | C2 | 2 | 2004 | 1127 | Ŕ | U 2 | 002-3 | 12358 | 30 | | : | 20010 | 201 | |
| US | 20040 | 1819 | 92 | | A1 | 2 | 2004 | 0129 | U | S 2 | 002- | 1815 | 52 | | : | 20020 | 718 | < |
| NO | 20020 | 0368 | 38 | | Α | 2 | 2002 | 1003 | N | 0 2 | 002-3 | 3688 | | | | 20020 | 802 | < |
| US | 20051 | 17671 | 12 | | A1 | 2 | 2005 | 0811 | U | S 2 | 005-9 | 97218 | 3 | | : | 20050 | 404 | < |
| PRIORITY | APPI | N. | INFO | . : | | | • | | J | P 2 | 000-2 | 26080 |) | | A : | 20000 | 203 | |
| | | | | | | | | | J | P 2 | 000-4 | 1020 | 34 | | A : | 20001 | 228 | |
| | | | , | | | | | | W | 0 2 | 001-3 | JP713 | 3 | 1 | W : | 20010 | 201 | |
| | | | | | | | | | U | S 2 | 002-3 | 18156 | 52 | | A1 2 | 20020 | 718 | |
| | | | | | | | | | | | | | | | | | | |

OTHER SOURCE(S): MARPAT 135:175421

Integrin expression inhibitors and remedies for arteriosclerosis, psoriasis, cancer, retinal angiogenesis, diabetic retinitis or inflammatory diseases, anticoagulant agents and cancerous metastasis inhibitors based on the integrin inhibitory effect. Namely, integrin expression inhibitors containing as the active ingredient sulfonamide compds. represented by the following general formula BKSO2N(R1)ZR, pharmacol. acceptable salts thereof or hydrates of the same wherein B represents optionally substituted C6-10 aryl or 6- to 10-membered heteroaryl wherein the ring may be partly saturated; K represents a single bond, -CH=CH- or -(CR4bR5b)mb- (wherein R4b and R5b may be the same or different and each represents hydrogen or C1-4 alkyl; and mb represents an integer of 1 or 2); R1 represents hydrogen or C1-6 alkyl; Z represents a single bond or CO-NH-; and R represents optionally substituted C6-10 aryl or 6- to 10-membered heteroaryl wherein the ring may be partly saturated IT 165668-28-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (integrin expression inhibitors for medical uses)

RN 165668-28-0 HCAPLUS

CN Benzenesulfonamide, N-(2,3-dihydro-2-oxo-1H-indol-7-yl)-4-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:526062 HCAPLUS

DOCUMENT NUMBER: 135:107328

TITLE: Preparation of 1,2-diarylbenzimidazolealkanoates and

analogs for treatment of disorders mediated by

microglia activation

INVENTOR(S): Kuhnke, Joachim; Halfbrodt, Wolfgang; Moenning, Ursula

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 141 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PA' | PATENT NO. | | | | | KIND DATE | | | i | APPL | ION : | | | | | | | |
|---------|------------------------------|-------|------|-----|--------------|-----------|-------|-------|-----|------|-------|-------|------------------|-----|------|------|------|---------|
| WO | 2001 | | | | A1 | | 2001 | 0719 | , | WO 2 | 001- | EP33 | 4 | | 2 | 0010 | 112 | <i></i> |
| | | | | | | | , AU, | | | | | | | | | | | |
| | | CR, | CU, | cz. | DK. | DM | , DZ, | EE. | ES. | FI. | GB. | GD. | GE. | GH. | GM. | HR. | HII. | |
| | | | | | | | , KE, | | | | | | | | | | | |
| | | LV, | MA, | MD, | MG, | MK | , MN, | MW, | MX, | MZ. | NO. | NZ. | PL. | PT. | RO. | RU. | SD. | |
| | | | | | | | TJ, | | | | | | | | | | | |
| | RW: | | | | | | , MZ, | | | | | | | | | | | |
| | | DE, | DK, | ES, | FI, | FR | GB, | GR, | IE, | IT, | LU, | MC. | NL. | PT. | SE. | TR. | BF. | |
| | | ВJ, | CF, | CG, | CI, | CM | GA, | GN, | GW, | ML, | MR, | NE, | SN, | TD, | TG | , | , | |
| CA | 2396 | 227 | | | A1 | | 2001 | 0719 | | CA 2 | 001- | 2396: | 227 [°] | • | 2 | 0010 | 112 | < |
| BR | 2396 2001 | 0076 | 28 | | Α | | 2002 | 1008 |] | BR 2 | 001- | 7628 | | | 2 | 0010 | 112 | < |
| EP | 1246 | 808 | | | A1 | | 2002 | 1009 |] | EP 2 | 001- | 9151 | 33 | | 2 | 0010 | 112 | < |
| | R: | ΑT, | BE, | CH, | DE, | DK. | , ES, | FR, | GB, | GR, | IT, | LI, | LU, | NL, | SE, | MC, | PT, | |
| | | ΙE, | SI, | LT, | LV, | FI, | , RO, | MK, | CY, | AL, | TR | | | | | · | | |
| HU | 2002 | 0401 | 1 | | A2 | | 2003 | 0528 | 1 | HU 2 | 002- | 4011 | | | 2 | 0010 | 112 | |
| JP | 2002 2002 5193 7829 | 5239 | 61 | | \mathbf{T} | | 2003 | 0812 | | JP 2 | 001- | 5518 | 55 | | 2 | 0010 | 112 | |
| EE | 2002 | 0039 | 0 | | Α | | 2003 | 1015 |] | EE 2 | 002- | 390 | | | 2 | 0010 | 112 | |
| NZ | 5193 | 26 | | | Α | | 2005 | 0225 | 1 | NZ 2 | 001- | 5193 | 26 | | 2 | 0010 | 112 | |
| AU | 7829 | 93 | | | B2 | | 2005 | 0915 | 7 | AU 2 | 001- | 4233 | 2 | | 2 | 0010 | 112 | |
| US | 2002 | 00694 | 48 | | A1 | | 2002 | 0117 | Ţ | JS 2 | 001- | 7593 | 60 | | 2 | 0010 | 116 | < |
| | 7115 | | | | | | 2006 | | | | | | | | | | | |
| IN | 2002 | MN00 | 672 | | A | | 2005 | 0304 | | IN 2 | 002-1 | MN67 | 2 | | 2 | 0020 | 524 | |
| BG | 1068 2002 | 21 | | | Α | | 2003 | 0131 | 1 | 3G 2 | 002- | 1068 | 21 | | 2 | 0020 | 613 | |
| NO | 2002 | 0033 | 52 | | Α | | 2002 | | 1 | 10 2 | 002- | 3362 | | | 2 | 0020 | 712 | < |
| | 2002 | - | _ | | | | 2004 | 0219 | | | | 6470 | | | | | | |
| | 2006 | | | | | | 2006 | | | | | 2991 | | | | | | |
| | 2006 | | | | A1 | | 2006 | 0914 | | | | 3055 | | | | | | < |
| RIORITY | Y APP | LN. | INFO | . : | | | | | I | DE 2 | 000- | 1000 | 2898 | Ž | A 2 | 0000 | 114 | |
| | | | | | | | | | Ţ | JS 2 | 000- | 1783 | 24P | 1 | P 2 | 0000 | 127 | |
| | | | | | | | | | I | NO 2 | 001- | EP33 | 4 | 1 | ₩ 2 | 0010 | 112 | |
| | | | | | | | | | | JS 2 | 001- | 7593 | 60 | 7 | A3 2 | 0010 | 116 | |
| THER SO | OURCE | (S): | | | MARI | PAT | 135: | 10732 | 28 | | | | | | | | | |

GI

$$\begin{array}{c|c}
R^3 & & \\
N & & R^2 \\
R & & R^1 & I
\end{array}$$

AB Title compds. [I; R = ZZ1R4; R1, R2 = (un) substituted (hetero) aryl; R3 = H, halo, substituted alkyl, alkoxy, etc.; R4 = CO2H, alkoxycarbonyl, CONH2, SO3H, etc.; Z = O, (alkyl)imino, acylimino; Z1 = (heteroatom-interrupted) alkyl(en)ylene, etc.] were prepared Thus, I (R1 = R2 = Ph, R3 = H)(II; R = 6-OH) was etherified by BrCH2CO2CHMe3 to give II (R = 6-OCH2CO2CHMe3). Data for biol. activity of I were given. 350232-45-0P 350232-47-2P 350232-48-3P 350232-49-4P 350232-50-7P 350232-51-8P 350232-52-9P 350232-53-0P 350232-55-2P 350232-92-7P 350232-94-9P 350232-98-3P 350233-00-0P 350233-04-4P 350233-08-8P 350233-12-4P 350233-16-8P 350234-15-0P 350234-18-3P 350234-19-4P 350234-22-9P 350234-25-2P 350234-28-5P 350234-29-6P 350234-31-0P 350234-32-1P 350234-34-3P 350234-35-4P 350234-36-5P 350234-37-6P 350234-38-7P 350234-48-9P 350234-53-6P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 1,2-diarylbenzimidazolealkanoates and analogs for treatment of disorders mediated by microglia activation)

Hexanoic acid, 6-[[5-[[(4-bromophenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

350232-45-0 HCAPLUS

RN -CN

RN 350232-47-2 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350232-48-3 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 350232-49-4 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]- (9CI) (CA INDEX NAME)

RN 350232-50-7 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(3-methylphenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 350232-51-8 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-methylphenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 350232-52-9 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-methoxyphenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 350232-53-0 HCAPLUS

CN Hexanoic acid, 6-[[1,2-diphenyl-5-[[[4-(trifluoromethyl)phenyl]sulfonyl]am ino]-1H-benzimidazol-6-yl]oxy]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 350232-55-2 HCAPLUS

CN Hexanoic acid, 6-[[5-[[[4-(acetylamino)phenyl]sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 350232-92-7 HCAPLUS

CN Benzenesulfonamide, N-(1,2-diphenyl-1H-benzimidazol-5-yl)- (9CI) (CA INDEX NAME)

RN 350232-94-9 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-(1,2-diphenyl-1H-benzimidazol-5-yl)- (9CI) (CA INDEX NAME)

RN 350232-98-3 HCAPLUS

CN Benzenesulfonamide, 4-chloro-N-(1,2-diphenyl-1H-benzimidazol-5-yl)- (9CI) (CA INDEX NAME)

RN 350233-00-0 HCAPLUS

CN Benzenesulfonamide, 4-bromo-N-(1,2-diphenyl-1H-benzimidazol-5-yl)- (9CI) (CA INDEX NAME)

RN 350233-04-4 HCAPLUS

CN Benzenesulfonamide, N-(1,2-diphenyl-1H-benzimidazol-5-yl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 350233-08-8 HCAPLUS

CN Benzenesulfonamide, N-(1,2-diphenyl-1H-benzimidazol-5-yl)-3-methyl- (9CI) (CA INDEX NAME)

RN 350233-12-4 HCAPLUS

CN Benzenesulfonamide, N-(1,2-diphenyl-1H-benzimidazol-5-yl)-4-methyl- (9CI) (CA INDEX NAME)

RN 350233-16-8 HCAPLUS

CN Benzenesulfonamide, N-(1,2-diphenyl-1H-benzimidazol-5-yl)-4-methoxy- (9CI) (CA INDEX NAME)

RN 350234-15-0 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1-(3,4-dimethylphenyl)-2-phenyl-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-18-3 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-2-(4-fluorophenyl)-1-(4-methoxyphenyl)-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-19-4 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1,2-bis(4-methoxyphenyl)-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-22-9 HCAPLUS

CN Butanoic acid, 4-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1-(4-methoxyphenyl)-2-phenyl-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-25-2 HCAPLUS

CN Pentanoic acid, 5-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1-(4-methoxyphenyl)-2-phenyl-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-28-5 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1-(4-methoxyphenyl)-2-phenyl-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-29-6 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1-(4-methoxyphenyl)-2-phenyl-1H-benzimidazol-6-yl]oxy]- (9CI) (CA INDEX NAME)

RN 350234-31-0 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1-(4-methylphenyl)-2-phenyl-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-32-1 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1-(4-methylphenyl)-2-phenyl-1H-benzimidazol-6-yl]oxy]- (9CI) (CA INDEX NAME)

RN 350234-34-3 HCAPLUS

CN Pentanoic acid, 5-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-35-4 HCAPLUS

CN Pentanoic acid, 5-[[5-[[(4-chlorophenyl)sulfonyl]amino]-1,2-diphenyl-1H-benzimidazol-6-yl]oxy]- (9CI) (CA INDEX NAME)

RN 350234-36-5 HCAPLUS

CN Hexanoic acid, 6-[[5-[[(4-fluorophenyl)sulfonyl]amino]-1-(4-methoxyphenyl)-2-phenyl-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-37-6 HCAPLUS

CN Hexanoic acid, 6-[[1-(4-methoxyphenyl)-2-phenyl-5-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 350234-38-7 HCAPLUS

CN Hexanoic acid, 6-[[1-(4-methoxyphenyl)-2-phenyl-5-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-benzimidazol-6-yl]oxy]- (9CI) (CA INDEX NAME)

RN 350234-48-9 HCAPLUS

CN Benzenesulfonamide, N-(1,2-diphenyl-1H-benzimidazol-5-yl)-4-fluoro- (9CI) (CA INDEX NAME)

RN 350234-53-6 HCAPLUS

CN Benzenesulfonamide, 4-chloro-N-[1-(4-methoxyphenyl)-2-phenyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2001:338351 HCAPLUS

DOCUMENT NUMBER:

134:340508

TITLE:

Preparation of 2-benzyl and 2-heteroaryl benzimidazole

NMDA/NR2B antagonists

INVENTOR(S):

McCauley, John A.; Theberge, Cory R.; Liverton, Nigel

J.; Claremon, David A.; Claiborne, Christopher F.

PATENT ASSIGNEE(S):

Merck & Co., Inc., USA PCT Int. Appl., 80 pp.

SOURCE: CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

GI

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT | NO. | | | KIND DATE | | | | | | | | DATE | | | | | |
|--------------|--------|--------|-----|-----------|-----|------|------|-----|-------|-------|----------|------|-----|------------|------|-------|--|
| WO 200 | 10321 | 74 | | A1 | - | 2001 | 0510 | | | | US29 | | | 20001026 < | | | |
| W: | ΑE, | AG, | AL, | AM, | ΑT, | AU, | ΑZ, | BA, | BB, | BG, | BR, | BY, | ΒZ, | CA, | CH, | CN, | |
| | | | | | | | | | | | GB, | | | | | | |
| | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KR, | KZ, | LC, | LK, | LR, | LS, | LT, | LU, | |
| | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NO, | NZ, | PL, | PT, | RO, | RU, | SD, | |
| | SE, | SG, | SI, | SK, | SL, | TJ, | TM, | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VN, | YU, | |
| | ZA, | ZW, | AM, | ΑZ, | BY, | KG, | ΚZ, | MD, | RU, | ТJ, | TM | | | | | | |
| RV | : GH, | GM, | ΚE, | LS, | MW, | MZ, | SD, | SL, | SZ, | TZ, | UG, | ZW, | AT, | BE, | CH, | CY, | |
| | DE, | DK, | ES, | FI, | FR, | GB, | GR, | ΙE, | IT, | LU, | MC, | NL, | PT, | SE, | BF, | ВJ, | |
| | CF, | CG, | CI, | CM, | GΑ, | GN, | GW, | ML, | MR, | NE, | SN, | TD, | TG | | | | |
| US 631 | 6474 | | | B1 | | 2001 | 1113 | | US 2 | 000- | 6965 | 01 | | 20 | 0001 | 025 < | |
| CA 238 | 9259 | | | A1 | | 2001 | 0510 | | CA 2 | 000- | 2389 | 259 | | 20 | 0001 | 026 < | |
| EP 124 | 2076 | | | A1 | | 2002 | 0925 | | EP 2 | 000- | 9753 | 93 | | 20 | 0001 | 026 < | |
| R: | ΑT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR, | IT, | LI, | LU, | NL, | SE, | MC, | PT, | |
| | ΙE, | SI, | LT, | LV, | FI, | RO, | MK, | CY, | AL | | | | | | | | |
| JP 200 | 351304 | 41 | | T | į | 2003 | 0408 | | JP 2 | 001- | 5343 | 79 | | 20 | 0001 | 026 | |
| PRIORITY A | PLN. | INFO | . : | | | • | | | US 19 | 999- | 1623 | 51P | 1 | P 19 | 9991 | 029 | |
| | | | | | | | | 1 | WO 2 | 000-1 | US29 | 470 | 1 | N 20 | 0001 | 026 | |
| OTHER SOURCE | E(S): | | | MAR | PAT | 134: | 3405 | 80 | | | | | | | | | |

$$R^{2}$$
 H
 R^{3}
 R^{4}
 R^{5}
 I

AB Novel benzimidazoles, substituted in the 2-position by substituted benzyl groups or heteroaryl groups, (I) [wherein R1, R2, R4, and R5 = independently H, Cl, F, OH, OMe, CF3, OCF3, NH2, CN, NO2, (amino)alkyl, aryl, alkylcarbonylamino, oxohydroxydibenzopyranyl-substituted carboxyphenylthioureido or carbonylaminoalkylcarbonylamino, R6SO2NH, R6SO2NMe, or R6SO2NHCH2; R3 = H, OH, NH2, alkylamino, arylamino, or :0; R6 = (un)substituted alkyl, (phenyl)alkenyl, Ph, naphthyl, or heterocyclic group; Y = 0, NH, (CH2)nCO(CH2)n, or (CH2)nCHR3(CH2)n; n = 0-5; Ar may be substituted with 0-3 N atoms in positions 2, 3, 5, or 6] were prepared as

RN

effective NMDA NR2B glutamate receptor antagonists. For example, cycloaddn. of phenylenediamine and (4-phenoxyphenyl)acetic acid in presence of EDC and HOBt in DMF afforded 2-(4-phenoxybenzyl)-1H-benzimidazole. Exptl. protocols for assessing the inhibition of NR1A/2B NMDA receptor activation (FLIPR assay) and determining the apparent dissociation

consts. against the human NR1A/NR2B receptor (binding assay) are given (no data). I are useful for relieving pain and treating depression, schizophrenia, Parkinson's disease, or stroke (no data).

IT 337965-02-3P 337965-03-4P 337965-05-6P 337965-07-8P 337965-09-0P 337965-11-4P 337965-13-6P 337965-15-8P 337965-17-0P 337965-19-2P 337965-21-6P 337965-23-8P 337965-25-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-benzyl and 2-heteroaryl benzimidazole NMDA/NR2B antagonists by cycloaddn. of phenylenediamines with arylacetates) 337965-02-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl](9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ O & & & \\ Ph-S-NH & & \\ O & & \\ O & & \\ \end{array}$$

RN 337965-03-4 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-02-3 CMF C26 H21 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 337965-05-6 HCAPLUS

Benzenesulfonamide, 2-methyl-N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-04-5 CMF C27 H23 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-07-8 HCAPLUS

CN Benzenesulfonamide, 3-methyl-N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-06-7 CMF C27 H23 N3 O3 S

Me
$$S-NH$$
 H CH_2 OPh

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-09-0 HCAPLUS

CN Benzenesulfonamide, 4-methyl-N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-08-9 CMF C27 H23 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-11-4 HCAPLUS

CN Benzenesulfonamide, 3-chloro-N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-10-3 CMF C26 H20 Cl N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-13-6 HCAPLUS

CN Benzenesulfonamide, 4-chloro-N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-12-5 CMF C26 H20 Cl N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-15-8 HCAPLUS

CN Benzenesulfonamide, 2-fluoro-N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-14-7 CMF C26 H20 F N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-17-0 HCAPLUS

CN Benzenesulfonamide, 4-fluoro-N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-16-9 CMF C26 H20 F N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-19-2 HCAPLUS

CN Benzenesulfonamide, 4-methoxy-N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-18-1 CMF C27 H23 N3 O4 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-21-6 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-20-5 CMF C27 H20 F3 N3 O4 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 337965-23-8 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-2-

(trifluoromethyl) -, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-22-7

CMF C27 H20 F3 N3 O3 S

$$\begin{array}{c|c} CF_3 & O & H & CH_2 \\ \hline & S - NH & N & CH_2 \\ \hline & O & N & N \\ \hline \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 337965-25-0 HCAPLUS

Benzenesulfonamide, N-[2-[(4-phenoxyphenyl)methyl]-1H-benzimidazol-5-yl]-4-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 337965-24-9

CMF C27 H20 F3 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 9 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:224233 HCAPLUS

DOCUMENT NUMBER: 134:252337

TITLE: Preparation of N-[(amindinophenethyl)benzimidazolyl]be

nzenesulfonamides and analogs as tryptase inhibitors
INVENTOR(S):
Anderskewitz, Ralf; Braun, Christine; Briem, Hans;
Disse, Bernd; Hoenke, Christoph; Jennewein, Hans

Michael; Speck, Georg

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany

SOURCE:

Ger. Offen., 28 pp.

CODEN: GWXXBX

DOCUMENT TYPE: LANGUAGE: Patent German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | | | | | KIND DATE | | | 7 | APPL | ICAT: | DATE | | | | | | |
|------------|---------------|------|------|-----|-------------|-----|------|------|------|-------|-------|-------|------|------------|------|-------|----------|
| | | | | | | - | | | - | | | | | | - | | |
| DE | 1994 | 5810 | | | A1 | | 2001 | 0329 | I | DE 19 | 999- | 1994 | 5810 | | 1: | 9990 | 924 < |
| CA | CA 2382892 | | | | | | | | (| CA 20 | 000-2 | 2382 | | 20000921 < | | | |
| WO | WO 2001023359 | | | | | | | | | | | | | | | | |
| | | | | | | | CN, | | | | | | | | | | |
| | | | | | | | | | | | | | | | | | ZA, |
| | | | | | | | MD, | | | | • | | • | | • | • | • |
| | RW: | | | | | | DK, | | | | GB, | GR, | IE, | IT. | LU. | MC. | NL. |
| | | PT, | | | | | • | • | • | • | | • | • | , | | | , |
| US | 6413 | 990 | | | B1 | | 2002 | 0702 | τ | JS 20 | 000-6 | 6667 | 69 | | 2 | 0000 | 921 < |
| | 1220 | | | | | | | | | | | | | | | | 921 < |
| EP | 1220 | 845 | | | B1 20030813 | | | | | | | | | | | | |
| | R: | AT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR, | IT, | LI, | LU, | NL. | SE. | MC. | PT. |
| | | | | | | | RO, | | • | • | • | • | • | • | | | , |
| JP | 2003 | 5103 | 09 | | T | | 2003 | 0318 | Ċ | JP 20 | 001-9 | 5265 | 13 | | 20 | 0000 | 921 |
| AT | 2470 | 92 | | | ${f T}$ | | 2003 | 0815 | I | AT 20 | 000-9 | 9692 | 75 | | 20 | 0000 | 921 |
| PRIORIT | Y APP | LN. | INFO | . : | | | | | Ι | DE 19 | 999- | 1994! | 5810 | | A 19 | 9990 | 924 |
| | | | | | | | | | τ | JS 19 | 999-: | 1573 | 89P | | P 19 | 9991 | 001 |
| | | | | | | | | | V | IO 20 | 000-I | EP92 | 36 | | | 20000 | |
| OTHER S | OURCE | (S): | | | MAR | PAT | 134: | 2523 | 37 | | | | | | | | |

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Title compds. (I; R5 = CH2CH2C6H4R2-4) [II; R = NR4SO2R3; R1 = (cyclo)alkyl, (un)substituted phenylalkyl, etc.; R2 = C(:NH)NH2 or CH2NH2; R3 = (un)substituted Ph, -naphthyl, -(benzo)thienyl, etc.; R4 = H, aminoalkyl, ureidoalkyl, etc.] were prepared Thus, 2-fluoro-5-nitroaniline was aminated and the product cyclocondensed with 4-(NC)C6H4CH2CH2CO2H to give, after reduction, II (R1 = Me)(III; R = NH2, R2 = cyano) which was amidated and the product converted in 4 steps to III [R =

4-(MeO2C)C6H4SO2N(CH2CH2NEt2), R2 = C(:NH)NH2]. Data for biol. activity of I were given.

IT 331449-67-3P 331449-68-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-[(amindinophenethyl)benzimidazolyl]benzenesulfonamides and analogs as tryptase inhibitors)

RN 331449-67-3 HCAPLUS

CN Benzoic acid, 4-[[[2-[2-(4-cyanophenyl)ethyl]-1-methyl-1H-benzimidazol-5-yl]amino]sulfonyl]- (9CI) (CA INDEX NAME)

$$HO_2C$$
 O
 S
 N
 CH_2
 CH_2
 O
 Me

RN 331449-68-4 HCAPLUS

CN Benzoic acid, 4-[[[2-[2-(4-cyanophenyl)ethyl]-1-methyl-1H-benzimidazol-5-yl]amino]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

L15 ANSWER 10 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:224232 HCAPLUS

DOCUMENT NUMBER: 134:266307

TITLE: Preparation of 2-arylethyl-5-

arylsulfonamidobenzimidazoles as tryptase inhibitors. INVENTOR(S): Anderskewitz, Ralf; Braun, Christine; Briem, Hans;

Disse, Bernd; Hoenke, Christoph; Jennewein, Hans

Michael; Speck, Georg

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany

SOURCE: Ger. Offen., 36 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND DATE | APPLICATION NO. | DATE |
|----------------|-------------------|-------------------------|-------------|
| | | | |
| DE 19945787 | A1 20010329 | DE 1999-19945787 | 19990924 < |
| CA 2379557 | A1 20010405 | CA 2000-2379557 | 20000921 < |
| WO 2001023360 | A1 20010405 | WO 2000-EP9237 | 20000921 < |
| W: AE, AU, BG, | , BR, CA, CN, CZ, | EE, HR, HU, ID, IL, IN, | JP, KR, LT, |

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LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, ZA,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
     US 6365584
                                 20020402
                                             US 2000-666765
                                                                     20000921 <--
     EP 1220844
                                                                     20000921 <--
                          A1
                                 20020710
                                             EP 2000-960686
     EP 1220844
                          B1
                                 20030409
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, CY
     JP 2003510310
                          Т
                                 20030318
                                             JP 2001-526514
                                                                     20000921
     AT 236887
                          Т
                                 20030415
                                             AT 2000-960686
                                                                     20000921
     PT 1220844
                          Т
                                 20030829
                                             PT 2000-960686
                                                                     20000921
     ES 2192543
                          Т3
                                 20031016
                                             ES 2000-960686
                                                                     20000921
PRIORITY APPLN. INFO.:
                                             DE 1999-19945787
                                                                  Α
                                                                     19990924
                                             US 1999-157278P
                                                                  Ρ
                                                                     19991001
                                             WO 2000-EP9237
                                                                  W
                                                                     20000921
OTHER SOURCE(S):
                         MARPAT 134:266307
GI
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$$\mathbb{R}^{3} SO_{2}^{N}_{R^{4}}$$

AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, phenylalkyl, heterocyclyl, heterocyclylalkyl; R2 = C(:NH)NH2, CH2NH2; R3 = Ph, PhCH2, naphthyl, furyl, benzofuryl, thienyl, benzothienyl; R4 = H, (substituted) alkyl, heterocyclyl, heterocyclylalkyl, etc.], were prepared Thus, N-[3-amino-4-(3,5-bistifluoromethylbenzylamino)phenyl]benzenesulfonamide (preparation given), p-cyanophenylpropionic acid, and POCl3 were heated together for 2 h at 100-120° to give 71.5% N-[2-[2-(4-cyanophenyl)ethyl]-1-(3,5-bistrifluoromethylbenzyl)benzimidazol-5-yl]benzenesulfonamide. This was stirred with HCl in EtOH at 0-5° and the residue after distillation of EtOH was treated with NH3 in EtOH to give 70.3% N-[2-[2-(4-amidinophenyl)ethyl]-1-(3,5-bistrifluoromethylbenzyl)benzimidazol-5-yl]benzenesulfonamide. I inhibited tryptase with IC50 = 0.0066-0.412 μM.

IT 331766-13-3P 331766-20-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of arylethylarylsulfonamidobenzimidazoles as tryptase inhibitors)

RN 331766-13-3 HCAPLUS

CN Benzenecarboximidamide, 4-[2-[1-[[3,5-bis(trifluoromethy1)pheny1]methy1]-5-[(phenylsulfony1)amino]-1H-benzimidazol-2-y1]ethy1]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ \parallel & \\ \text{C-NH}_2 \\ \\ \text{R---CH}_2 - \text{CH}_2 - \text{CH}_2 \end{array}$$

• HCl

RN 331766-20-2 HCAPLUS

CN Benzenecarboximidamide, 4-[2-[1-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \parallel \\ Ph-S-NH \\ \parallel \\ O \end{array}$$

$$\begin{array}{c} CF_3 \\ \parallel \\ CF_2 \end{array}$$

$$CF_3$$

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{C-NH}_2 \end{array}$$
 R—CH₂-CH₂-CH₂-

IT 256493-19-3P 331766-54-2P 331766-59-7P

331766-62-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of arylethylarylsulfonamidobenzimidazoles as tryptase inhibitors)

RN 256493-19-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[2-(4-cyanophenyl)ethyl]-1-methyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ Ph-S-NH & & & \\ O & & & \\ \end{array}$$

RN 331766-54-2 HCAPLUS

CN Benzenesulfonamide, N-[1-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-[2-(4-cyanophenyl)ethyl]-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$R - CH_2 - CH_2$$

RN 331766-59-7 HCAPLUS

CN Benzenesulfonamide, N-[2-[2-(4-cyanophenyl)ethyl]-1-(3-ethoxypropyl)-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Ph-S-NH \\ O \\ \end{array}$$

$$\begin{array}{c} CH_2-CH_2 \\ \end{array}$$

$$\begin{array}{c} CH_2-CH_2 \\ \end{array}$$

$$\begin{array}{c} CH_2-CH_2 \\ \end{array}$$

RN - 331766-62-2 HCAPLUS

CN Benzenecarboximidamide, N-hydroxy-4-[2-[1-methyl-5-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Ph-S-NH \\ O \\ \end{array}$$

L15 ANSWER 11 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:790487 HCAPLUS

DOCUMENT NUMBER: 133:335229

TITLE: Preparation of benzoxazole compounds, process for the

preparation thereof and herbicides

INVENTOR(S): Fukuda, Shohei; Nakamura, Akira; Shimizu, Motohisa;

Okada, Tatsuo; Asahara, Takehiko; Oohida, Satoshi

PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND DATE | APPLICATION NO. | DATE | | | | |
|------------------------|------------------|---------------------|-----------------|--|--|--|--|
| | | | - | | | | |
| WO 2000066569 | A1 20001109 | WO 2000-JP2760 | 20000427 < | | | | |
| W: BR, CA, CN, | IN, US | | | | | | |
| RW: AT, BE, CH, | CY, DE, DK, ES, | FI, FR, GB, GR, IE, | IT, LU, MC, NL, | | | | |
| PT, SE | | | | | | | |
| CA 2371681 | A1 20001109 | CA 2000-2371681 | 20000427 < | | | | |
| JP 2001011061 | A 20010116 | JP 2000-126933 | 20000427 < | | | | |
| BR 2000010703 | A 20020219 | BR 2000-10703 | 20000427 < | | | | |
| EP 1180515 | A1 20020220 | EP 2000-921051 | 20000427 < | | | | |
| EP 1180515 | B1 20040414 | | | | | | |
| R: AT, BE, CH, | DE, DK, ES, FR, | GB, GR, IT, LI, LU, | NL, SE, MC, PT, | | | | |
| IE, FI | | | | | | | |
| AT 264314 | T 20040415 | AT 2000-921051 | 20000427 | | | | |
| ES 2219332 | T3 20041201 | ES 2000-921051 | 20000427 | | | | |
| US 6706664 | B1 20040316 | US 2001-959544 | 20011030 < | | | | |
| PRIORITY APPLN. INFO.: | | JP 1999-124912 | A 19990430 | | | | |
| | | WO 2000-JP2760 | W 20000427 | | | | |
| OTHER SOURCE(S): | MARPAT 133:33522 | .9 | | | | | |

AB Claimed are benzoxazole compds. represented by general formula (I; wherein R1 to R4 are each hydrogen, C1-6 alkyl, C1-4 alkoxy, C1-4 haloalkyl, C1-4 haloalkoxy, halogeno, nitro, cyano, or the like; R5 is C1-4 haloalkyl, C1-4 haloalkoxy, halogeno, nitro, cyano, or the like; R6 is hydrogen, halogeno, cyano, nitro, or the like; R7 is hydrogen, C1-6 alkyl, C1-4 haloalkyl, or the like; and X is O, S, SO, or SO2); process for the preparation of them; and herbicides containing the same as the active ingredient. Thus, chlorination of 2-[4-fluoro-3-(trifluoromethyl)phenoxy]butanoic acid with SOC12 under reflux for 2 h gave 2-[4-fluoro-3-

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(trifluoromethyl)phenoxy]butanoyl chloride which underwent cyclocondensation with 2-amino-4-fluorophenol in AcOH at 50-60° for 1 h to give 1-(5-fluorobenzoxazol-2-yl)-1-[4-fluoro-3-(trifluoromethyl)phenoxy]propane (II). II at 500 g/ha (preemergent soil-treatment) completely controlled Digitaria ciliaris, Echinochloa crus-galli, Setaria viridis, and Poa annua and gave no damage to corn, soy bean, cotton, and wheat plants.

IT 303183-23-5P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of benzoxazole compds., process for preparation thereof and herbicides)

RN 303183-23-5 HCAPLUS

CN Benzenesulfonamide, N-[2-[1-[4-fluoro-3-(trifluoromethyl)phenoxy]propyl]-5benzoxazolyl]-4-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 12 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2000:83221 HCAPLUS

DOCUMENT NUMBER:

132:137386

TITLE:

Preparation of heterocyclylalkylbenzamidines and

analogs as thrombin inhibitors

INVENTOR(S):

Hauel, Norbert; Ries, Uwe; Priepke, Henning; Mihm, Gerhard; Wienen, Wolfgang; Stassen, Jean Marie;

Binder, Klaus; Zimmermann, Rainer

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma K.-G., Germany

SOURCE:

Ger. Offen., 58 pp.

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND DATE | APPLICATION NO. | DATE |
|-----------------|---------------|---------------------------|-----------------|
| | | | |
| DE 19834751 | A1 200002 | 203 DE 1998-19834751 | 19980801 < |
| US 6121308 | A 200009 | 919 US 1999-359487 | 19990722 < |
| CA 2337825 | A1 200002 | 217 CA 1999-2337825 | 19990727 < |
| WO 2000008014 | A1 200002 | 217 WO 1999-EP5371 | 19990727 < |
| W: AE, AL, AM, | AT, AU, AZ, B | BA, BB, BG, BR, BY, CA, | CH, CN, CU, CZ, |
| DE, DK, EE, | ES, FI, GB, G | GD, GE, GH, GM, HR, HU, | ID, IL, IN, IS, |
| JP, KE, KG, | KP, KR, KZ, L | CC, LK, LR, LS, LT, LU, 1 | LV, MD, MG, MK, |
| MN, MW, MX, | NO, NZ, PL, P | PT, RO, RU, SD, SE, SG, | SI, SK, SL, TJ, |
| TM, TR, TT, | UA, UG, UZ, V | N, YU, ZA, ZW | |
| RW: GH, GM, KE, | LS, MW, SD, S | SL, SZ, UG, ZW, AT, BE, G | CH, CY, DE, DK, |
| ES, FI, FR, | GB, GR, IE, I | [T, LU, MC, NL, PT, SE,] | BF, BJ, CF, CG, |
| CI, CM, GA, | GN, GW, ML, M | MR, NE, SN, TD, TG | |
| AU 9952885 | A 200002 | 228 AU 1999-52885 | 19990727 < |

| EP | 1100 | 795 | | | A1 | | 2001 | 0523 | I | ΞP | 1999- | 9383 | 53 | | 1 | 9990 | 727 | < |
|----------|-------|-------|------|-----|------|------|------|------|-----|------|-------|------|------|-----|-----|-------|-----|---|
| EP | 1100 | 795 | | | B1 | | 2004 | 0609 | | | | | | | | | | |
| | R: | AT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR | , IT, | LI, | LU, | NL, | SE, | MC, | PT. | |
| | | | | | LV, | | | | - | | | • | | • | • | • | • | |
| JP | 2002 | 5224 | 32 | | T | | 2002 | 0723 | j | JP : | 2000- | 5636 | 47 | | 1 | 9990 | 727 | < |
| AT | 2687 | 63 | | | T | | 2004 | 0615 | Į | Υ | 1999- | 9383 | 53 | | 1 | 9990 | 727 | |
| PT | 1100 | 795 | | | T | | 2004 | 1029 | I | PT | 1999- | 9383 | 53 | | 1 | 99901 | 727 | |
| ES | 2223 | 177 | | | Т3 | | 2005 | 0216 | I | ES | 1999- | 9383 | 53 | | 1 | 9990 | 727 | |
| PRIORITY | APP | LN. | INFO | . : | | | | | Ι | ÞΕ | 1998- | 1983 | 4751 | 1 | 1 | 99808 | 301 | |
| | | | | | | | | | τ | JS | 1998- | 9883 | 8P | I | 2 1 | 99809 | 902 | |
| | | | | | | | | | V | O | 1999- | EP53 | 71 | V | V 1 | 99901 | 727 | |
| OTHER SC | MIRCE | (S) · | | | MADE | ידעכ | 132. | 1272 | 86 | | | | | | | | | |

OTHER SOURCE(S): MARPAT 132:137386
GI

$$^{\text{Me}}_{\text{O}}$$
 $^{\text{S}}_{\text{O}}$ $^{\text{NH}}_{\text{NH}_2}$ $^{\text{NH}}_{\text{II}}$

AB RaZ2Z1ZR [I; R = cyano or C(:NH)NHRb; Ra = (alkyl)amino, phenylalkoxy, NR4COR3, etc.; Rb = H, OH, alkyl, metabolically labile group; Z = (un)substituted (hetero)arylene; Z1 = (alkyl-substituted) CH2CH2, -OCH2, -CH2O, -NHCH2, etc.; Z2 = indole-, benzimidazole-, benzoxazole-n,2-diyl, quinolinediyl, etc.; n = 4-7] were prepared Thus, 2-methylamino-5-nitroaniline was cyclocondensed with HO2CCH2CH2C6H4(CN)-4 and the reduced product N-substituted by, successively, MeSO2Cl and BrCH2CO2Et to give, after aminolysis and saponification, title compound II. Data for biol. activity of

I were given.

IT 256491-55-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclylalkylbenzamidines and analogs as thrombin inhibitors)

RN 256491-55-1 HCAPLUS

CN Benzenecarboximidamide, 3-[[1-methyl-5-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]methoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Ph-S-NH \\ O \\ \end{array}$$

$$\begin{array}{c} N \\ N \\ \end{array}$$

$$\begin{array}{c} C-NH_2 \\ \\ NH \\ \end{array}$$

$$\begin{array}{c} C-NH_2 \\ \\ NH \\ \end{array}$$

IT 256493-19-3 256493-38-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heterocyclylalkylbenzamidines and analogs as thrombin inhibitors)

RN 256493-19-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[2-(4-cyanophenyl)ethyl]-1-methyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Ph-S-NH \\ O \\ \end{array}$$

$$\begin{array}{c} CN \\ CH_2-CH_2 \\ \end{array}$$

$$\begin{array}{c} CN \\ Me \\ \end{array}$$

RN 256493-38-6 HCAPLUS

CN Benzenesulfonamide, N-[2-[(3-cyanophenoxy)methyl]-1-methyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \parallel \\ Ph-S-NH \\ O \\ \end{array}$$

$$\begin{array}{c} N \\ \downarrow \\ CH_2-O \\ \end{array}$$

$$\begin{array}{c} CH_2-O \\ \end{array}$$

$$\begin{array}{c} CN \\ \end{array}$$

IT 256492-55-4P 256492-57-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocyclylalkylbenzamidines and analogs as thrombin inhibitors)

RN 256492-55-4 HCAPLUS

CN 1H-Benzimidazole-1-acetic acid, 2-[(4-cyanophenoxy)methyl]-5-[(phenylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ Ph-S-NH & & & \\ O & & & N \\ \hline \\ CH_2-C-OEt \\ \end{array}$$

RN 256492-57-6 HCAPLUS

CN 1H-Benzimidazole-1-acetic acid, 2-[(4-cyanophenoxy)methyl]-6-[(phenylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

L15 ANSWER 13 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1999:819384 HCAPLUS

DOCUMENT NUMBER:

132:64058

TITLE:

Preparation and antitumor activity of

arylsulfonanilide phosphates

INVENTOR(S):

Houze, Jonathan B.

PATENT ASSIGNEE(S):

Tularik Inc., USA

SOURCE:

PCT Int. Appl., 42 pp. CODEN: PIXXD2

VPE: Paten

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PA' | PATENT NO. | | | | | KIND DATE | | | | | ICAT | | | | | | | |
|---------|------------|------|------|-----|-----|-----------|-------|-------|-----|------|------|------------|-----|-----|------|------|-----|---|
| OW. | WO 9967258 | | | | | | | | | | | 19990616 < | | | | | | |
| | | | | | | | AZ, | | | | | | | | | | | ` |
| | | - | - | - | - | | GB, | | • | • | | | | | | | . , | |
| | | | | | | | KZ, | | | | | | | | | | | |
| , | | | | | | | PL, | | | | | | | | | | | |
| | | | | | | | , UZ, | | | | | | | | | | | |
| | | | TJ, | | | | | | | | | • | • | · | • | • | • | |
| | RW: | GH, | GM, | KE, | LS, | MW | , SD, | SL, | SZ, | ŪĠ, | ZW, | AT, | ΒE, | CH, | CY, | DE, | DK, | |
| | | ES, | FI, | FR, | GB, | GR, | , IE, | IT, | LU, | MC, | NL, | PT, | SE, | BF, | ВJ, | CF, | CG, | |
| | | CI, | CM, | GΑ, | GN, | GW, | , ML, | MR., | NE, | SN, | TD, | TG | | | | | | |
| CA | 2335 | 559 | | | A1 | | 1999 | 1229 | (| CA 1 | 999- | 2335 | 559 | | 1 | 9990 | 616 | < |
| | 9945 | | | | Α | | 2000 | 0110 | i | AU 1 | 999- | 4576 | 8 | | 1 | 9990 | 616 | < |
| | 7636 | | | | | | 2003 | | | | | | | | | | | |
| EP | 1090 | 014 | | | A1 | | 2001 | 0411 |] | EP 1 | 999- | 9287 | 77 | | 1 | 9990 | 616 | < |
| EP | 1090 | | | | | | 2003 | | | | | | | | | | | |
| | R: | | | CH, | DE, | DK, | , ES, | FR, | GB, | GR, | IT, | LI, | LU, | NL, | SE, | MC, | PT, | |
| | | ΙE, | | | | | | | | | | | | | | | | |
| | 2002 | | | | | | 2002 | 0625 | | JP 2 | 000- | 5559 | 10 | | 1 | 9990 | 616 | < |
| | 2488 | | | | Т | | 2003 | 0915 | i | AT 1 | 999- | 9287 | 77 | | 1 | 9990 | 616 | |
| | 6211 | | | | | | 2001 | 0403 | | | 000- | | | | | 0000 | 614 | < |
| | 2001 | | 30 | | | | 2001 | | Ţ | JS 2 | 001- | 7794 | 19 | | 2 | 0010 | 207 | < |
| | 6417 | | | | B2 | | 2002 | 0709 | | | | | | | | | | |
| RIORIT | APP: | LN. | INFO | .: | | | | | Ţ | JS 1 | 998- | 9068 | 1P |] | P 1 | 9980 | 625 | |
| | | | | | | | | | 1 | WO 1 | 999- | US13 | 759 | 1 | W 1 | 9990 | 616 | |
| | | | | | | | | | 1 | JS 1 | 999- | 3360 | 62 | 1 | B1 1 | 9990 | 618 | |
| | | | | | | | | | | JS 2 | 000- | 5953 | 98 | 7 | A1 2 | 0000 | 614 | |
| THER SO | OURCE | (S): | | | MAR | PAT | 132: | 64058 | 3 | | | | | | | | | |

TΤ

AB The title compds. I [R1 = H, alkyl, heteroalkyl; R2, R3 = H, halo, alkyl, etc.; R2 and R3 when attached to adjacent C atoms can form a ring; R4, R5 = H, alkyl, aryl, etc.; Ar = substituted Ph] were prepared and their antitumor activity assessed. E.g., 5-(pentafluorophenylsulfonamido)-2-methoxyphenyl phosphate was prepared

253141-42-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and antitumor activity of arylsulfonanilide phosphates)

RN 253141-42-3 HCAPLUS

CN Benzenesulfonamide, 2,3,4,5,6-pentafluoro-N-[7-(phosphonooxy)-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

Ι

$$F \longrightarrow F \longrightarrow O \longrightarrow M$$

$$F \longrightarrow O \longrightarrow M$$

$$OPO_3H_2$$

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 14 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1999:505930 HCAPLUS

DOCUMENT NUMBER:

131:157761

TITLE:

5-Membered heterocyclic condensed benzo derivatives,

their preparation, and their use as drugs

INVENTOR(S):

Ries, Uwe; Hauel, Norbert; Mihm, Gerhard; Priepke,

Henning; Binder, Klaus; Stassen, Jean Marie; Wienen,

Wolfgang; Zimmermann, Rainer

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma K.-G., Germany

SOURCE:

Ger. Offen., 94 pp. CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PAT | CENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----|----------|------|----------|------------------|------------|
| | | | | | |
| DE | 19804085 | A1 | 19990805 | DE 1998-19804085 | 19980203 < |
| CA | 2319494 | A1 | 19990812 | CA 1999-2319494 | 19990128 < |
| WO | 9940072 | A1 | 19990812 | WO 1999-EP537 | 19990128 < |

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AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
             KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN,
             MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
             TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
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     AU 9927201
                          Α
                                 19990823
                                             AU 1999-27201
                                                                     19990128 <--
     EP 1060166
                          A1
                                 20001220
                                             EP 1999-907437
                                                                     19990128 <--
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     JP 2002502844
                          T
                                 20020129
                                             JP 2000-530502
                                                                     19990128 <--
     US 6114532
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                                 20000905
                                             US 1999-243200
                                                                     19990202 <--
PRIORITY APPLN. INFO.:
                                             DE 1998-19804085
                                                                    19980203
                                                                  Α
                                             US 1998-77694P
                                                                     19980312
                                                                  Р
                                             DE 1998-19834325
                                                                  Α
                                                                    19980730
                                             WO 1999-EP537
                                                                    19990128
                                                                  W
OTHER SOURCE(S):
                         MARPAT 131:157761
     Approx. 300 antithrombotic title compds. such as 4-[5-[N-(8-
     quinolylsulfonyl) -N-(carboxymethyl)amino]-1-methyl-1H-benzimidazol-2-
     ylmethyl]benzamidine hydrochloride (I), 4-[5-[N-(benzenesulfonyl)-N-[2-
     (dimethylamino) ethyl] amino] -1-benzyl-1H-benzimidazol-2-
     ylmethyl]benzamidine dihydrochloride, 4-[5-[N-(3-carboxypropionyl)-N-
     (cyclopentyl) amino] -1-methyl-1H-benzimidazol-2-ylmethyl] benzamidine
     hydrochloride (II), and 4-[5-[N-(8-quinolylsulfonyl)-N-
     (carboxymethyl) amino] -1-methyl-1H-benzothiazol-2-ylmethyl]benzamidine
     hydrochloride were prepared by standard methods. The ED200 in µM for I was
     0.92 and for II was 0.82. Formulations for the antithrombotics were
     given.
     236418-60-3 237750-73-1 237750-74-2
     237750-75-3 237750-76-4 237750-77-5
     237750-78-6 237750-80-0 237750-86-6
     237750-87-7 237750-88-8 237750-92-4
     237751-01-8 237751-21-2 237752-02-2
     237752-09-9 237752-10-2 237752-11-3
     237752-12-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation and antithrombotic activity of benzimidazolylmethylbenzamidines
RN
     236418-60-3 HCAPLUS
     1H-Benzimidazole-1-acetic acid, 2-[(4-cyanophenyl)methyl]-5-
CN
     [(phenylsulfonyl)amino] - (9CI) (CA INDEX NAME)
Ph-S
      - NH
                       H_2 - CO_2H
```

Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1H-benzimidazol-5-yl]-

(9CI)

237750-73-1 HCAPLUS

(CA INDEX NAME)

RN

CN

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 237750-74-2 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-7-methyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \parallel \\ Ph-S-NH \\ \parallel \\ O \\ \hline \\ Me \\ \end{array}$$

RN 237750-75-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-6-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 237750-76-4 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-propyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ Ph-S-NH & & & \\ O & & & N \end{array}$$

RN 237750-77-5 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-propyl-1H-benzimidazol-6-yl]- (9CI) (CA INDEX NAME)

RN 237750-78-6 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-ethyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

RN 237750-80-0 HCAPLUS

CN 1H-Benzimidazole-1-acetic acid, 2-[(4-cyanophenyl)methyl]-5-[(phenylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 237750-86-6 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl]-3,5-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$F_3C$$
 CF_3
 CH_2
 CN
 CH_2
 Me

RN 237750-87-7. HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl]-2,5-dimethoxy- (9CI) (CA INDEX NAME)

RN 237750-88-8 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl]-2,3,5,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 237750-92-4 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-4-yl]- (9CI) (CA INDEX NAME)

RN 237751-01-8 HCAPLUS

CN Benzoic acid, 3-[[[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl]amino]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 237751-21-2 HCAPLUS

CN 1H-Benzimidazole-1-propanoic acid, 2-[(4-cyanophenyl)methyl]-5-[(phenylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 237752-02-2 HCAPLUS

CN 1H-Benzimidazole-1-acetic acid, 2-[(4-cyanophenyl)methyl]-6-[(phenylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 237752-09-9 HCAPLUS

CN 1H-Benzimidazole-1-butanoic acid, 2-[(4-cyanophenyl)methyl]-5-[(phenylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 237752-10-2 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-(phenylmethyl)-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \parallel \\ Ph-S-NH \\ \parallel \\ O \end{array}$$

$$CH_2-Ph$$

RN 237752-11-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-[2-(4-morpholinyl)ethyl]-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ Ph-S-NH & & & \\ \hline \\ O & & & \\ \end{array}$$

RN 237752-12-4 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-[2-(dimethylamino)ethyl]-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Ph-S-NH \\ O \\ \end{array}$$

$$CH_2-CH_2-NMe_2$$

IT 236414-44-1P 236417-29-1P 236417-38-2P

236418-28-3P 237750-36-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and antithrombotic activity of benzimidazolylmethylbenzamidines

RN 236414-44-1 HCAPLUS

CN 1H-Benzimidazole-1-acetic acid, 2-[[4-(aminoiminomethyl)phenyl]methyl]-5[(phenylsulfonyl)amino]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH & NH \\ \parallel & C-NH_2 \\ \hline O & N & O \\ \hline CH_2-C-OEt \end{array}$$

HC1

RN 236417-29-1 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Ph-S-NH \\ O \\ \end{array}$$

$$\begin{array}{c} O \\ N \\ \end{array}$$

$$\begin{array}{c} CN \\ \end{array}$$

RN 236417-38-2 HCAPLUS

CN Glycine, N-[[2-[(4-cyanophenyl)methyl]-5-[(phenylsulfonyl)amino]-1H-benzimidazol-1-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 236418-28-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)methyl]-5-benzoxazolyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & CH_2 \\ \hline O & NH \\ \hline O & N \\ \hline \end{array}$$

RN 237750-36-6 HCAPLUS

CN Benzoic acid, 3-[[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]amino]sulfonyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} & \text{NH} \\ & \text{C} & \text{NH}_2 \\ & \text{C} & \text{NH}_2 \\ &$$

HCl

$$\begin{array}{c} O \\ | \\ Ph-S-NH \\ | \\ O \end{array}$$

$$\begin{array}{c} NH \\ | \\ C-NH_2 \end{array}$$

$$\begin{array}{c} NH \\ | \\ C-NH_2 \end{array}$$

$$\begin{array}{c} NH \\ | \\ C-NH_2 \end{array}$$

HCl

RN 236414-29-2 HCAPLUS
CN Benzenecarboximidamide, 4-[[5-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{C-NH}_2 \\ \\ \text{Ph-} & \\ \text{S-NH} \\ \\ \text{O} \end{array}$$

HCl

RN 236414-31-6 HCAPLUS
CN Benzenecarboximidamide, 4-[[4-methyl-6-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} & \text{NH} \\ & \text{C-NH}_2 \\ & \text{NH} & \text{CH}_2 \\ &$$

HCl

RN 236414-32-7 HCAPLUS

CN Benzenecarboximidamide, 4-[[1-methyl-6-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} & \\ & \text{NH} \\ & \text{C-NH}_2 \\ \\ \text{Ph-S-NH} & \\ & \text{Me} \\ \\ & \text{O} \end{array}$$

● HCl

RN 236414-34-9 HCAPLUS

CN Benzenecarboximidamide, 4-[[5-[(phenylsulfonyl)amino]-1-propyl-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH & NH \\ \parallel & C-NH_2 \\ \hline O & N & Pr-n \end{array}$$

→ HCl

RN 236414-36-1 HCAPLUS

CN Benzenecarboximidamide, 4-[[6-[(phenylsulfonyl)amino]-1-propyl-1H-

03/13/2007

benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & NH & NH & NH \\ \hline 0 & & & CH_2 & \\ Ph-S-NH & & & Pr-n \\ \hline 0 & & & & \\ & & & & \\ & & & & \\ \end{array}$$

HC1

RN 236414-40-7 HCAPLUS

CN Benzenecarboximidamide, 4-[[1-ethyl-5-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ | \\ Ph-S-NH \\ | \\ O \end{array}$$

$$\begin{array}{c} NH \\ | \\ C-NH_2 \\ \\ Et \end{array}$$

● HCl

RN 236414-45-2 HCAPLUS

CN 1H-Benzimidazole-1-acetic acid, 2-[[4-(aminoiminomethyl)phenyl]methyl]-5-[(phenylsulfonyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH & NH \\ \parallel & C-NH_2 \\ \hline O & N & CH_2-CO_2H \end{array}$$

RN 236414-55-4 HCAPLUS

CN Benzenecarboximidamide, 4-[[5-[[[3,5-bis(trifluoromethyl)phenyl]sulfonyl]a mino]-1-methyl-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 236414-56-5 HCAPLUS

CN Benzenecarboximidamide, 4-[[5-[[(2,5-dimethoxyphenyl)sulfonyl]amino]-1-methyl-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

OMe
$$CH_2$$
 $C-NH_2$
OMe NH

● HCl

RN 236414-57-6 HCAPLUS CN Benzenecarboximidamic

Benzenecarboximidamide, 4-[[1-methyl-5-[[(2,3,5,6-tetramethylphenyl)sulfonyl]amino]-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{NH} \\ & \text{Me} & \text{O} \\ & \text{S} & \text{NH} \\ & \text{O} & \text{N} \\ & \text{Me} & \text{Me} \\ \end{array}$$

• HCl

RN 236414-63-4 HCAPLUS

CN Benzenecarboximidamide, 4-[[1-methyl-4-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH & NH \\ \parallel & \parallel & \parallel \\ O & N & \parallel & \parallel \\ O & N & CH_2 & Me \end{array}$$

● HCl

RN 236414-87-2 HCAPLUS

CN Benzoic acid, 3-[[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]amino]sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 236415-07-9 HCAPLUS

CN 1H-Benzimidazole-1-butanoic acid, 2-[[4-(aminoiminomethyl)phenyl]methyl]-5-[(phenylsulfonyl)amino]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH & NH \\ \parallel & C-NH_2 \\ \hline O & N & O \\ \hline & (CH_2)_3-C-OEt \end{array}$$

● HCl

RN 236415-08-0 HCAPLUS

CN Benzenecarboximidamide, 4-[[1-(phenylmethyl)-5-[(phenylsulfonyl)amino]-1H-

03/13/2007

benzimidazol-2-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Ph-S-NH \\ O \\ \end{array}$$

$$CH_2-Ph$$

● HCl

RN 236415-09-1 HCAPLUS

CN Benzenecarboximidamide, 4-[[1-[2-(4-morpholinyl)ethyl]-5-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH \\ \parallel & C-NH_2 \\ \hline O & N-CH_2-CH_2-N \\ \hline \end{array}$$

●2 HCl

RN 236415-10-4 HCAPLUS

CN Benzenecarboximidamide, 4-[[1-[2-(dimethylamino)ethyl]-5-[(phenylsulfonyl)amino]-1H-benzimidazol-2-yl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \text{Ph-S-NH} \\ \text{O} \\ \text{O} \\ \text{CH}_2\text{-CH}_2\text{-NMe}_2 \end{array}$$

●2 HCl

RN 236415-53-5 HCAPLUS

CN 1H-Benzimidazole-1-propanoic acid, 2-[[4-(aminoiminomethyl)phenyl]methyl]5-[(phenylsulfonyl)amino]-, ethyl ester, monohydrochloride (9CI) (CA
INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & \\ & & & & & & \\ Ph-S-NH & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\$$

HCl

RN 236416-84-5 HCAPLUS

CN Benzenecarboximidamide, 4-[[5-[(phenylsulfonyl)amino]-2-benzoxazolyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & NH & NH & NH \\ & & C-NH_2 \\ & & C-NH_2 \\ & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & &$$

● HCl

RN 237750-37-7 HCAPLUS

CN 1H-Benzimidazole-1-acetic acid, 2-[[4-(aminoiminomethyl)phenyl]methyl]-6[(phenylsulfonyl)amino]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

L15 ANSWER 15 OF 39 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1999:35065 HCAPLUS

DOCUMENT NUMBER:

130:110166

TITLE:

Preparation of amidinophenylpropionyltetrahydroquinoli

nes and related compounds as antithrombotics.

INVENTOR(S):

Heckel, Armin; Soyka, Rainer; Grell, Wolfgang; Haaksma, Eric; Binder, Klaus; Zimmermann, Rainer

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma K.-G., Germany

SOURCE:

Ger. Offen., 50 pp. CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PA' | PATENT NO. | | | | | | | | APPL | ICAT | ION 1 | | DATE | | | | | | |
|----------|------------|------|------|-----|-----|------|------|------|------|-------------|----------|------|----------|------------|------------|-------|-------|---|--|
| DE | 1972 | | | | | | 1999 | 0107 | 1 | DE 1 | 997- | 1972 | 7117 | | 19970626 < | | | | |
| CA | CA 2288744 | | | Δ1 | | | | | | | | | | | | | | | |
| | WO 9900371 | | | | | | | | | | | | | 19980622 < | | | | | |
| "" | | | | | | | | | | | | | | | | | | | |
| | VV . | | | | | | BA, | | | | | | | | | | | | |
| | | | | | | | GE, | | | | | | | | | | | | |
| | | | | | | | LR, | | | | | | | | | | | | |
| | | | | | | | RU, | | | | | | | | | | | | |
| | | | | | | | YU, | | | | | | | | | | | | |
| | RW: | GH, | GM, | KΕ, | LS, | MW, | SD, | SZ, | ŬĠ, | ZW, | ΑT, | BE, | CH, | CY, | DE, | DK, | ES, | | |
| | | FI, | FR, | GB, | GR, | ΙE, | IT, | LU, | MC, | NL, | PT, | SE, | BF, | ВJ, | CF, | CG, | CI, | | |
| | | | | | | | NE, | | | | | | _ | | | | • | • | |
| AU | 98872 | | | | | | 1999 | | | | 998- | 8727 | 9 | | 1 | 9980 | 622 | < | |
| EP | 99162 | 24 | | | | | | | | | | | | | | | | | |
| | 99162 | | | | | | 2003 | | | | | | | | _ | | | | |
| | R: | AT. | | | | | ES, | | | GR | TT | T.T | T.JT | MT. | SE | MC | рт | | |
| | | IE, | | , | 22, | 210, | 20, | , | CD, | 010, | , | шт, | ш, | ип, | 55, | nc, | Ε . , | | |
| J.T. | 20029 | | | | т | | 2002 | 0400 | | TD 1 | 000_ | 5052 | 6 | | 1 | 9980 | 622 | | |
| | 25460 | | - | | T | | 2002 | | | | | | | | _ | 9980 | | ζ | |
| | 99112 | | | | _ | | | - | | | | | | | | | | | |
| | | | | | A | | 2000 | | | | | 1126 | | | | 99912 | | | |
| | 63003 | | | | В1 | | 2001 | 1009 | | | | | | | | 99912 | | < | |
| PRIORITY | Y APPI | LN. | INFO | .: | | | | | | | | | | | | 99706 | | | |
| | | | | | | | | | 1 | NO 1 | 998-1 | EP38 | 00 | 1 | W 1: | 99806 | 522 | | |
| OTHER SO | OURCE | (S): | | | MAR | PAT | 130: | 1101 | 66 | | | | | | | | | • | |

OTE

GI

AB Title compds. [I; Ra = H, NO2, amino, aminocarbonyl; Rb = cyano, aminomethyl, (substituted) amidino; Rc, Rd = H, F, Cl, Br, iodo, Me, MeO, NO2, amino; A = (substituted) ethylene, ethyenylene, propylene, etc.; B = bond, (substituted) methylene, ethylene, ethenylene, propylene, etc.; W = N, CH; Y = CH2, CO, CS], were prepared Thus, 1-[3-(4-amidinophenyl)propionyl]-1,2,3,4-tetrahydroquinoline-6-carboxylic acid methyl-N-phenylamide (preparation given) had a thrombin time ED200 = 0.02 µM.

IT 219643-32-0P 219644-16-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amidinophenylpropionyltetrahydroquinolines and related compds. as antithrombotics)

RN 219643-32-0 HCAPLUS

CN 1H-Indol-5-amine, 1-[3-(4-cyanophenyl)-1-oxopropyl]-2,3-dihydro-N-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ Ph-S-NH & & & & \\ O & & & & \\ O & & & & \\ \end{array}$$

RN 219644-16-3 HCAPLUS

CN 1H-Indol-5-amine, 1-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-2,3-dihydro-N-(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH & NH \\ Ph-S-NH & O & C-NH_2 \\ \hline O & N-C-CH_2-CH_2 \\ \end{array}$$

● HCl

=> log y COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

136.81

700.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

CA SUBSCRIBER PRICE

ENTRY -17.94

SESSION -20.28

STN INTERNATIONAL LOGOFF AT 12:58:14 ON 13 MAR 2007